

## SEARCH REQUEST FORM

Scientific and Technical Information Center

Requester's Full Name: Robert (Rex) Shaw Examiner #: 79521 Date: 2/14/05  
 Art Unit: 1626 Phone Number: 2-0909 Serial Number: 10/628,394  
 Mail Box and Bldg/Room Location: 5A10/5C18 Results Format Preferred (circle): PAPER DISK E-MAIL

If more than one search is submitted, please prioritize searches in order of need. MEY

\*\*\*\*\*  
 Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc. if known. Please attach a copy of the cover sheet, pertinent claims, and abstract.

Title of invention:

Methods for protecting an optical beta-amino acid

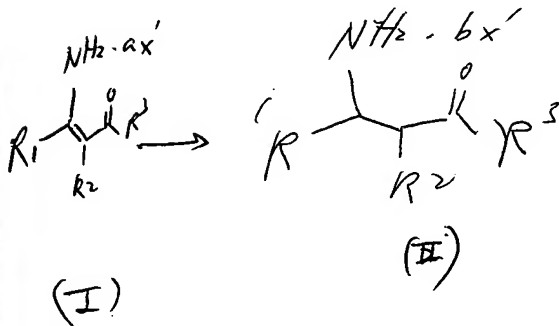
Inventors (please provide full names):

Hatsumi et al.

Earliest Priority Filing Date: \_\_\_\_\_

\*For Sequence Searches Only\* Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.

2 search a prior for info cpd by

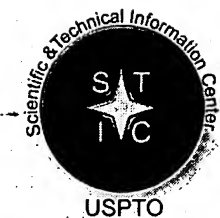
\* R<sub>1</sub> R<sub>2</sub> R<sub>3</sub> are sub

\* ax' is 0, or 1,

\* X is acid

## STAFF USE ONLY

Searcher: <u>Thibbe</u>	Type of Search	Vendors and cost where applicable
Searcher Phone # _____	NA Sequence (#) _____	STN <u>414</u>
Searcher Location: _____	AA Sequence (#) _____	Dialog _____
Date Searcher Picked Up: _____	Structure (#) <u>1</u>	Questel/Orbit _____
Date Completed: <u>2/23/05</u>	Bibliographic <u>/</u>	Dr. Link _____
Searcher Prep. Review Time <u>10</u>	Litigation _____	Lexis/Nexis _____
Clerical Prep. Time: _____	Fulltext _____	Sequence Systems _____
Online Time <u>20</u>	Patent Family _____	WWWinternet _____
	Other _____	Other (specify) _____



# **STIC Search Report**

## **Biotech-Chem Library**

**STIC Database Tracking Number: 145081**

**TO: Rei-Tsang Shiao**  
**Location: 5a10 / 5c18**  
**Art Unit: 1626**  
**Wednesday, February 23, 2005**

**Case Serial Number: 10/628394**

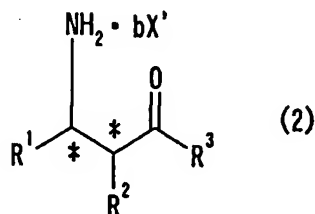
**From: Noble Jarrell**  
**Location: Biotech-Chem Library**  
**Rem 1B71**  
**Phone: 272-2556**

**Noble.jarrell@uspto.gov**

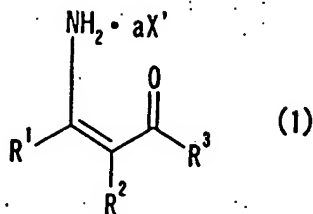
### **Search Notes**

## Amendments to the Claims

1. (Original) A method for producing an optically active  $\beta$ -amino acid of formula (2),



, wherein b is 0 or 1; the symbol \* shows that the carbon atom is a chiral carbon; R<sup>1</sup> is a hydrogen atom, an alkyl group, a substituted alkyl group, a cycloalkyl group, a substituted cycloalkyl group, an aralkyl group, a substituted aralkyl group, an aryl group, a substituted aryl group, an aliphatic heterocyclic group, a substituted aliphatic heterocyclic group, an aromatic heterocyclic group, a substituted aromatic heterocyclic group, an alkoxy group, a substituted alkoxy group, an aralkyloxy group, a substituted aralkyloxy group, an aryloxy group or a substituted aryloxy group; R<sup>2</sup> is a hydrogen atom, an alkyl group, a substituted alkyl group, a cycloalkyl group, a substituted cycloalkyl group, an aralkyl group, a substituted aralkyl group, an aryl group, a substituted aryl group, an aliphatic heterocyclic group, a substituted aliphatic heterocyclic group, an aromatic heterocyclic group, a substituted aromatic heterocyclic group, an alkoxy group, a substituted alkoxy group, an aralkyloxy group, a substituted aralkyloxy group, an aryloxy group, a substituted aryloxy group, an alkyloxycarbonyl group or an aralkyloxycarbonyl group; R<sup>3</sup> is an alkoxy group, a substituted alkoxy group, an aralkyloxy group, a substituted aralkyloxy group, an aryloxy group, a substituted aryloxy group, an amino group or a substituted amino group, X' is an acid, and R<sup>1</sup> and R<sup>2</sup> or R<sup>2</sup> and R<sup>3</sup> may be combined together to form a ring provided that R<sup>1</sup> and R<sup>2</sup> are not a hydrogen atom simultaneously, which comprises subjecting an enamine of formula (1),



, wherein  $\text{R}^1$ ,  $\text{R}^2$ ,  $\text{R}^3$  and  $\text{X}'$  have the same meanings as described above, and  $a$  is 0 or 1, to an asymmetric hydrogenation.

2. (Original) The method as claimed in claim 1, wherein the asymmetric hydrogenation is carried out in the presence of an acid.

3. (Original) The method as claimed in claim 1, wherein the asymmetric hydrogenation is carried out in the presence of a fluorine-containing aliphatic alcohol.

4. (Currently Amended) The method as claimed in ~~any of~~ claims 1 to 3, wherein the asymmetric hydrogenation is carried out in the presence of a catalyst for the asymmetric hydrogenation.

5. (Original) The method as claimed in claim 4, wherein the catalyst for the asymmetric hydrogenation is a transition metal complex.

6. (Original) The method as claimed in claim 5, wherein the transition metal complex is a complex of a metal which belongs to the eighth group of the periodic table.

**7. (Currently Amended)** The method as claimed in ~~either claim 5 or claim 6~~, wherein the transition metal complex has a chiral ligand.

**8. (Original)** The method as claimed in claim 7, wherein the chiral ligand is a chiral phosphine ligand.

**9. (Original)** The method as claimed in claim 1, wherein the asymmetric hydrogenation is carried out in the presence of an acid and a fluorine-containing aliphatic alcohol.

**10. (New)** The method as claimed in claim 2, wherein the asymmetric hydrogenation is carried out in the presence of a catalyst for the asymmetric hydrogenation.

**11. (New)** The method as claimed in claim 3, wherein the asymmetric hydrogenation is carried out in the presence of a catalyst for the asymmetric hydrogenation.

**12. (New)** The method as claimed in claim 6, wherein the transition metal complex has a chiral ligand.

4.14 (dq, J=2.1, 7.1Hz, 2H), 4.72 (br t, J=7.2Hz, 1H),  
7.40-7.50 (m, 5H); <sup>13</sup>C-NMR (CD<sub>3</sub>OD): δ:14.3, 39.4, 39.5,  
53.1, 62.4, 128.3, 130.4, 130.6, 137.3, 171.2; EI-MS (m/z):  
194 ([M]<sup>+</sup>)

5

#### Example 9

##### Production of methyl (S)-3-aminobutanoate

Under a nitrogen atmosphere, 78.0 mg (0.0869 mmol)  
of Ru(OCOCH<sub>3</sub>)<sub>2</sub>((S)-tol-binap), 1.00g (8.69 mmol) of methyl  
10 3-aminocrotonate and 5 ml of 2,2,2-trifluoroethanol were  
placed in a stainless steel autoclave, and the mixture was  
kept at 50 °C under 3MPa pressure of hydrogen for 15 hours  
with stirring. After completion of the reaction, the  
solvent was distilled off, and the residue was purified  
15 by a silica gel chromatography (eluent: ethyl acetate/  
methanol/ triethylamine = 95/5/5) to give the objective  
methyl (S)-3-aminobutanoate (0.149 g, pale yellow oil) in  
a yield of 14.6%.

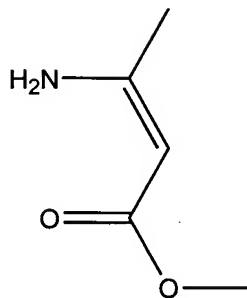
The enantiomeric excess was measured after  
20 conversion of the methyl (S)-3-aminobutanoate obtained  
into methyl (S)-3-acetamidobutanoate by acetylation with  
acetic anhydride in the presence of triethylamine, and was  
found to be 96.7%ee.

25

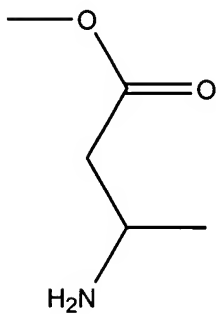
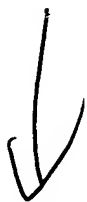
#### Example 10

##### Production of methyl (S)-3-aminobutanoate

The reaction was carried out in a manner similar to  
that in Example 9, except that 35.5 mg (0.0217 mmol) of



methyl -3-aminocrotonate



methyl -3-aminobutanoate

*Sample*



## UNITED STATES PATENT AND TRADEMARK OFFICE

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**\*BIBDATASHEET\***

Bib Data Sheet

**CONFIRMATION NO. 3969**

SERIAL NUMBER 10/628,394	FILING DATE 07/29/2003  RULE	CLASS 548	GROUP ART UNIT 1626	ATTORNEY DOCKET NO. 2003_1003A
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## APPLICANTS

Kazuhiko Matsumura, Hiratsuka-shi, JAPAN;

 Xiaoyong Zhang, Hiratsuka-shi, JAPAN;  
 Takao Saito, Hiratsuka-shi, JAPAN;

\*\* CONTINUING DATA \*\*\*\*\*

\*\* FOREIGN APPLICATIONS \*\*\*\*\*

JAPAN 222149/2002 07/30/2002

IF REQUIRED, FOREIGN FILING LICENSE GRANTED

\*\* 10/29/2003

Foreign Priority claimed 35 USC 119 (a-d) conditions met Verified and Acknowledged	<input type="checkbox"/> yes <input type="checkbox"/> no <input type="checkbox"/> yes <input type="checkbox"/> no <input type="checkbox"/> Met after Allowance Examiner's Signature _____ Initials _____	STATE OR  COUNTRY JAPAN	SHEETS  DRAWING 0	TOTAL  CLAIMS 12	INDEPENDENT  CLAIMS 1
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## ADDRESS

000513

WENDEROTH, LIND &amp; PONACK, L.L.P.

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SUITE 800

WASHINGTON, DC

20006-1021

## TITLE

Method for producing an optically active beta-amino acid

FILING FEE  RECEIVED 880	FEES: Authority has been given in Paper No. _____ to charge/credit DEPOSIT ACCOUNT No. _____ for following:	<input type="checkbox"/> All Fees <input type="checkbox"/> 1.16 Fees ( Filing ) <input type="checkbox"/> 1.17 Fees ( Processing Ext. of time ) <input type="checkbox"/> 1.18 Fees ( Issue ) <input type="checkbox"/> Other _____ <input type="checkbox"/> Credit
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E JP2002-222149/AP,PRN  
L2 1 JP2002-222149/AP,PRN  
L3 1 L1-2

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FILE 'HCAPLUS' ENTERED AT 08:22:34 ON 23 FEB 2005  
L4 TRA L3 1- RN : 28 TERMS

FILE 'REGISTRY' ENTERED AT 08:22:34 ON 23 FEB 2005  
L5 28 SEA L4

FILE 'WPIX' ENTERED AT 08:22:37 ON 23 FEB 2005  
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L7 1 JP2002-222149/AP,PRN  
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FILE COVERS 1907 - 23 Feb 2005 VOL 142 ISS 9  
FILE LAST UPDATED: 22 Feb 2005 (20050222/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

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L3 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2005 ACS on STN  
AN 2004:97223 HCAPLUS  
DN 140:128682  
ED Entered STN: 06 Feb 2004  
TI Method for producing an optically active .beta.-amino acid  
IN Matsumura, Kazuhiko; Zhang, Xiaoyong; Saito, Takao  
PA Takasago International Corporation, Japan  
SO Eur. Pat. Appl., 22 pp.  
CODEN: EPXXDW  
DT Patent  
LA English  
IC ICM C07B053-00  
ICS C07C227-32; C07C229-08  
CC 34-2 (Amino Acids, Peptides, and Proteins)

## FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 1386901	A1	20040204	EP 2003-16551	20030724 <--
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
	US 2004023344	A1	20040205	US 2003-628394	20030729 <--
	JP 2004075684	A2	20040311	JP 2003-282165	20030729 <--
PRAI	JP 2002-222149	A	20020730	<--	

## CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
EP 1386901	ICM	C07B053-00
	ICS	C07C227-32; C07C229-08
JP 2004075684	FTERM	4H006/AA02; 4H006/AC11; 4H006/AC81; 4H006/BA23; 4H006/BA32; 4H006/BA48; 4H006/BE20; 4H006/BJ50; 4H006/BT12; 4H006/BU32; 4H039/CA19; 4H039/CB10 <--

OS MARPAT 140:128682

AB Optically active .beta.-amino acids H<sub>2</sub>NCHR<sub>1</sub>CHR<sub>2</sub>COR<sub>3</sub> [R<sub>1</sub> is H, (un)substituted alkyl, cycloalkyl, aralkyl, aryl, heterocyclyl, alkoxy, aralkoxy, or aryloxy; R<sub>2</sub> is any group given for R<sub>1</sub> or (un)substituted alkoxy-carbonyl; R<sub>3</sub> is (un)substituted alkoxy, aralkoxy, aryloxy, or amino] and their salts, useful as intermediates for the production of medicines, agricultural chems. and physiol. active substances, were prepared by asym. hydrogenation of enamines H<sub>2</sub>NCR<sub>1</sub>:CR<sub>2</sub>COR<sub>3</sub> or their salts. Thus, Me 3-amino-3-phenylacrylate in MeOH was hydrogenated over Ru(OAc)<sub>2</sub>[(R)-H<sub>8</sub>-binap] in the presence of chloroacetic acid at 50.degree. and 3 MPa H<sub>2</sub> pressure for 88 h to afford 39.5% Me (S)-3-amino-3-phenylpropionate.

ST beta amino acid prepn asym hydrogenation enamine

IT Enamines

RL: RCT (Reactant); RACT (Reactant or reagent)  
(method for producing optically active .beta.-amino acids)

IT Hydrogenation

(stereoselective; method for producing optically active .beta.-amino acids)

IT Amino acids, preparation

RL: SPN (Synthetic preparation); PREP (Preparation)  
(.beta.-; method for producing optically active .beta.-amino acids)

IT 650601-38-0P

RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(method for producing optically active .beta.-amino acids)

IT 3082-68-6P 3082-69-7P 14553-88-9P 37088-66-7P 83509-89-1P  
650601-36-8P 650601-37-9P 650601-39-1P 650601-40-4P

RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)

(method for producing optically active .beta.-amino acids)

IT 94-02-0, Ethyl benzoylacetate 540-69-2, Ammonium formate 614-27-7, Methyl benzoylacetate 10472-24-9, Methyl 2 oxocyclopentanecarboxylate 14205-39-1, Methyl 3 aminocrotonate 36244-62-9 67354-34-1 134568-16-4

RL: RCT (Reactant); RACT (Reactant or reagent)

(method for producing optically active .beta.-amino acids)

IT 33831-72-0P 52909-60-1P 67654-59-5P 70272-01-4P 90956-83-5P  
288254-55-7P 650601-35-7P 650601-41-5P 650602-19-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(method for producing optically active .beta.-amino acids)

IT 650601-42-6P

RL: SPN (Synthetic preparation); PREP (Preparation)

(method for producing optically active .beta.-amino acids)

RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

- (1) Anon; PATENT ABSTRACTS OF JAPAN 1994, V018(680), PC-1291  
 (2) Daicel Chem Ind Ltd; JP 06271520 A 1994 HCAPLUS  
 (3) Heller, D; JOURNAL OF ORGANIC CHEMISTRY 2001, V66(20), P6816 HCAPLUS  
 (4) Penn State Res Found; WO 0240491 A 2002 HCAPLUS

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STRUCTURE FILE UPDATES: 22 FEB 2005 HIGHEST RN 835870-69-4  
 DICTIONARY FILE UPDATES: 22 FEB 2005 HIGHEST RN 835870-69-4

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 18, 2005

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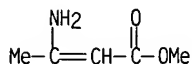
Experimental and calculated property data are now available. For more  
 information enter HELP PROP at an arrow prompt in the file or refer  
 to the file summary sheet on the web at:  
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=> d ide 15 tot

L5 ANSWER 1 OF 28 REGISTRY COPYRIGHT 2005 ACS on STN  
 RN 650602-19-0 REGISTRY  
 CN 2-Butenoic acid, 3-amino-, methyl ester, 4-methylbenzenesulfonate (9CI)  
 (CA INDEX NAME)  
 MF C7 H8 O3 S . C5 H9 N O2  
 SR CA  
 LC STN Files: CA, CAPLUS, USPATFULL  
 DT.CA CAplus document type: Patent  
 RL.P Roles from patents: PREP (Preparation); RACT (Reactant or reagent)

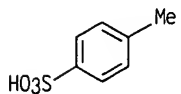
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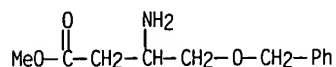
CM 2

CRN 104-15-4  
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1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L5 ANSWER 2 OF 28 REGISTRY COPYRIGHT 2005 ACS on STN  
RN 650601-42-6 REGISTRY  
CN Butanoic acid, 3-amino-4-(phenylmethoxy)-, methyl ester (9CI) (CA INDEX NAME)  
FS 3D CONCORD  
MF C12 H17 N O3  
SR CA  
LC STN Files: CA, CAPLUS, USPATFULL  
DT.CA CAplus document type: Patent  
RL.P Roles from patents: PREP (Preparation)



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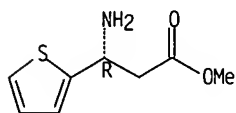
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1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L5 ANSWER 3 OF 28 REGISTRY COPYRIGHT 2005 ACS on STN  
RN 650601-41-5 REGISTRY  
CN 2-Thiophenepropanoic acid, .beta.-amino-, methyl ester, (.beta.R)-, methanesulfonate (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C8 H11 N O2 S . C H4 O3 S  
SR CA  
LC STN Files: CA, CAPLUS, USPATFULL  
DT.CA CAplus document type: Patent  
RL.P Roles from patents: PREP (Preparation); RACT (Reactant or reagent)

CM 1

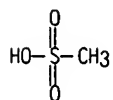
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CMF C8 H11 N O2 S

Absolute stereochemistry. Rotation (+).



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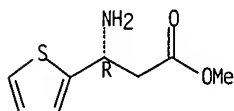


1 REFERENCES IN FILE CA (1907 TO DATE)

## 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L5 ANSWER 4 OF 28 REGISTRY COPYRIGHT 2005 ACS on STN  
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CN 2-Thiophenepropanoic acid, .beta.-amino-, methyl ester, (.beta.R)- (9CI)  
(CA INDEX NAME)  
FS STEREOSEARCH  
MF C8 H11 N O2 S  
CI COM  
SR CA  
LC STN Files: CA, CAPLUS, USPATFULL  
DT.CA CAplus document type: Patent  
RL.P Roles from patents: PREP (Preparation)

Absolute stereochemistry. Rotation (+).



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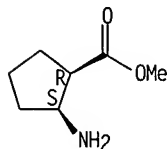
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1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

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RN 650601-39-1 REGISTRY  
CN Cyclopentanecarboxylic acid, 2-amino-, methyl ester, (1R-cis)-,  
methanesulfonate (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C7 H13 N O2 . C H4 O3 S  
SR CA  
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DT.CA CAplus document type: Patent  
RL.P Roles from patents: PREP (Preparation)

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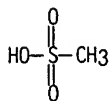
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Absolute stereochemistry. Rotation (-).



CM 2

CRN 75-75-2  
CMF C H4 O3 S



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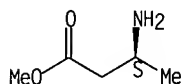
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1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L5 ANSWER 6 OF 28 REGISTRY COPYRIGHT 2005 ACS on STN  
RN 650601-38-0 REGISTRY  
CN Butanoic acid, 3-amino-, methyl ester, (3S)-, 4-methylbenzenesulfonate (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C7 H8 O3 S . C5 H11 N O2  
SR CA  
LC STN Files: CA, CAPLUS, USPATFULL  
DT.CA CAplus document type: Patent  
RL.P Roles from patents: PREP (Preparation); RACT (Reactant or reagent)

CM 1

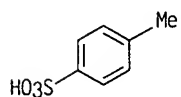
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Absolute stereochemistry.



CM 2

CRN 104-15-4  
CMF C7 H8 O3 S



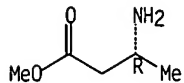
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1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L5 ANSWER 7 OF 28 REGISTRY COPYRIGHT 2005 ACS on STN  
RN 650601-37-9 REGISTRY  
CN Butanoic acid, 3-amino-, methyl ester, (3R)-, methanesulfonate (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C5 H11 N O2 . C H4 O3 S  
SR CA  
LC STN Files: CA, CAPLUS, USPATFULL  
DT.CA CAplus document type: Patent  
RL.P Roles from patents: PREP (Preparation)

CM 1

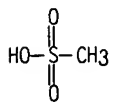
CRN 103189-63-5  
CMF C5 H11 N O2

Absolute stereochemistry. Rotation (-).



CM 2

CRN 75-75-2  
CMF C H4 O3 S



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

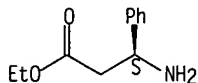
1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L5 ANSWER 8 OF 28 REGISTRY COPYRIGHT 2005 ACS on STN  
RN 650601-36-8 REGISTRY  
CN Benzenepropanoic acid, .beta.-amino-, ethyl ester, (.beta.S)-, methanesulfonate (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C11 H15 N O2 . C H4 O3 S  
SR CA  
LC STN Files: CA, CAPLUS, USPATFULL  
DT.CA CAplus document type: Patent  
RL.P Roles from patents: PREP (Preparation)

CM 1

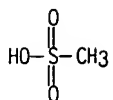
CRN 3082-69-7  
CMF C11 H15 N O2

Absolute stereochemistry. Rotation (+).



CM 2

CRN 75-75-2  
CMF C H4 O3 S

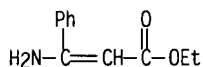


1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L5 ANSWER 9 OF 28 REGISTRY COPYRIGHT 2005 ACS on STN  
RN 650601-35-7 REGISTRY  
CN 2-Propenoic acid, 3-amino-3-phenyl-, ethyl ester, methanesulfonate (9CI)  
(CA INDEX NAME)  
MF C11 H13 N O2 . C H4 O3 S  
SR CA  
LC STN Files: CA, CAPLUS, USPATFULL  
DT.CA CAplus document type: Patent  
RL.P Roles from patents: PREP (Preparation); RACT (Reactant or reagent)

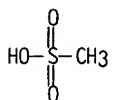
CM 1

CRN 33831-72-0  
CMF C11 H13 N O2



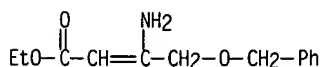
CM 2

CRN 75-75-2  
CMF C H4 O3 S



1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

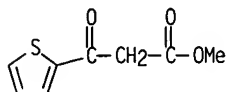
L5 ANSWER 10 OF 28 REGISTRY COPYRIGHT 2005 ACS on STN  
RN 288254-55-7 REGISTRY  
CN 2-Butenoic acid, 3-amino-4-(phenylmethoxy)-, ethyl ester (9CI) (CA INDEX NAME)  
FS 3D CONCORD  
MF C13 H17 N O3  
SR CA  
LC STN Files: CA, CAPLUS, USPATFULL  
DT.CA CAplus document type: Patent  
RL.P Roles from patents: PREP (Preparation); RACT (Reactant or reagent)



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2 REFERENCES IN FILE CA (1907 TO DATE)  
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

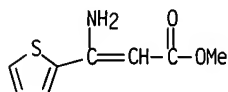
L5 ANSWER 11 OF 28 REGISTRY COPYRIGHT 2005 ACS on STN  
RN 134568-16-4 REGISTRY  
CN 2-Thiophenepropanoic acid, .beta.-oxo-, methyl ester (9CI) (CA INDEX NAME)  
OTHER NAMES:  
CN Methyl 3-oxo-3-(2-thienyl)propanoate  
FS 3D CONCORD  
MF C8 H8 O3 S  
SR CA  
LC STN Files: BEILSTEIN\*, CA, CAPLUS, CASREACT, CHEMCATS, USPATFULL  
(\*File contains numerically searchable property data)  
DT.CA CAplus document type: Journal; Patent  
RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); PROC (Process); RACT (Reactant or reagent)  
RL.NP Roles from non-patents: PREP (Preparation); RACT (Reactant or reagent)



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

14 REFERENCES IN FILE CA (1907 TO DATE)  
14 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L5 ANSWER 12 OF 28 REGISTRY COPYRIGHT 2005 ACS on STN  
RN 90956-83-5 REGISTRY  
CN 2-Propenoic acid, 3-amino-3-(2-thienyl)-, methyl ester (9CI) (CA INDEX NAME)  
FS 3D CONCORD  
MF C8 H9 N O2 S  
LC STN Files: CA, CAPLUS, USPATFULL  
DT.CA CAplus document type: Patent  
RL.P Roles from patents: PREP (Preparation); RACT (Reactant or reagent)



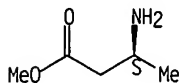
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

2 REFERENCES IN FILE CA (1907 TO DATE)  
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L5 ANSWER 13 OF 28 REGISTRY COPYRIGHT 2005 ACS on STN  
RN 83509-89-1 REGISTRY  
CN Butanoic acid, 3-amino-, methyl ester, (3S)- (9CI) (CA INDEX NAME)  
OTHER CA INDEX NAMES:  
CN Butanoic acid, 3-amino-, methyl ester, (S)-  
OTHER NAMES:  
CN Methyl (S)-3-aminobutanoate  
FS STEREOSEARCH

MF C5 H11 N O2  
 CI COM  
 LC STN Files: BEILSTEIN\*, CA, CAPLUS, CASREACT, CHEMINFORMRX, TOXCENTER, USPATFULL  
 (\*File contains numerically searchable property data)  
 DT.CA CAplus document type: Journal; Patent  
 RL.P Roles from patents: PREP (Preparation); RACT (Reactant or reagent)  
 RL.NP Roles from non-patents: ANST (Analytical study); PREP (Preparation); PROC (Process); RACT (Reactant or reagent)

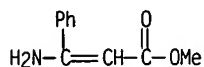
Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

13 REFERENCES IN FILE CA (1907 TO DATE)  
 13 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L5 ANSWER 14 OF 28 REGISTRY COPYRIGHT 2005 ACS on STN  
 RN 70272-01-4 REGISTRY  
 CN 2-Propenoic acid, 3-amino-3-phenyl-, methyl ester (9CI) (CA INDEX NAME)  
 FS 3D CONCORD  
 MF C10 H11 N O2  
 LC STN Files: BEILSTEIN\*, CA, CAPLUS, CASREACT, TOXCENTER, USPATFULL  
 (\*File contains numerically searchable property data)  
 DT.CA CAplus document type: Journal; Patent  
 RL.P Roles from patents: PREP (Preparation); RACT (Reactant or reagent)  
 RLD.P Roles for non-specific derivatives from patents: RACT (Reactant or reagent)  
 RL.NP Roles from non-patents: PREP (Preparation); RACT (Reactant or reagent)

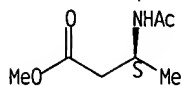


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

8 REFERENCES IN FILE CA (1907 TO DATE)  
 1 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA  
 8 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L5 ANSWER 15 OF 28 REGISTRY COPYRIGHT 2005 ACS on STN  
 RN 67654-59-5 REGISTRY  
 CN Butanoic acid, 3-(acetamino)-, methyl ester, (3S)- (9CI) (CA INDEX NAME)  
 OTHER CA INDEX NAMES:  
 CN Butanoic acid, 3-(acetamino)-, methyl ester, (S)-  
 OTHER NAMES:  
 CN N-((S)-3-Methoxy-1-methyl-3-oxopropyl)acetamide  
 FS STEREOSEARCH  
 MF C7 H13 N O3  
 LC STN Files: BEILSTEIN\*, CA, CAPLUS, CASREACT, CHEMINFORMRX, USPATFULL  
 (\*File contains numerically searchable property data)  
 DT.CA CAplus document type: Journal; Patent  
 RL.P Roles from patents: PREP (Preparation); RACT (Reactant or reagent)  
 RL.NP Roles from non-patents: PREP (Preparation); USES (Uses)

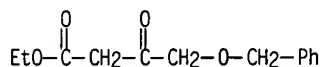
Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

22 REFERENCES IN FILE CA (1907 TO DATE)  
22 REFERENCES IN FILE CAPLUS (1907 TO DATE)

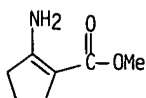
L5 ANSWER 16 OF 28 REGISTRY COPYRIGHT 2005 ACS on STN  
RN 67354-34-1 REGISTRY  
CN Butanoic acid, 3-oxo-4-(phenylmethoxy)-, ethyl ester (9CI) (CA INDEX NAME)  
OTHER NAMES:  
CN 4-Benzyloxyacetoacetic acid ethyl ester  
CN Ethyl 3-oxo-4-(phenylmethoxy)butanoate  
CN Ethyl 4-(benzyloxy)acetoacetate  
CN Ethyl 4-benzyloxy-3-oxobutanoate  
CN Ethyl 4-benzyloxy-3-oxobutyrate  
FS 3D CONCORD  
MF C13 H16 O4  
LC STN Files: BEILSTEIN\*, BIOBUSINESS, CA, CAPLUS, CASREACT, TOXCENTER, USPATFULL  
(\*File contains numerically searchable property data)  
DT.CA Caplus document type: Conference; Journal; Patent  
RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)  
RLD.P Roles for non-specific derivatives from patents: BIOL (Biological study); PROC (Process); RACT (Reactant or reagent)  
RL.NP Roles from non-patents: BIOL (Biological study); PREP (Preparation); PROC (Process); RACT (Reactant or reagent)



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

53 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA  
53 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L5 ANSWER 17 OF 28 REGISTRY COPYRIGHT 2005 ACS on STN  
RN 52909-60-1 REGISTRY  
CN 1-Cyclopentene-1-carboxylic acid, 2-amino-, methyl ester (9CI) (CA INDEX NAME)  
OTHER NAMES:  
CN Methyl 2-amino-1-cyclopentenecarboxylate  
FS 3D CONCORD  
MF C7 H11 N O2  
LC STN Files: BEILSTEIN\*, CA, CAPLUS, CASREACT, IFICDB, IFIPAT, IFIUDB, TOXCENTER, USPATFULL  
(\*File contains numerically searchable property data)  
DT.CA Caplus document type: Journal; Patent  
RL.P Roles from patents: PREP (Preparation); RACT (Reactant or reagent)  
RL.NP Roles from non-patents: PREP (Preparation); PRP (Properties)

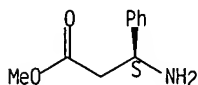


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

7 REFERENCES IN FILE CA (1907 TO DATE)  
7 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L5 ANSWER 18 OF 28 REGISTRY COPYRIGHT 2005 ACS on STN  
RN 37088-66-7 REGISTRY  
CN Benzenepropanoic acid, .beta.-amino-, methyl ester, (.beta.S)- (9CI) (CA INDEX NAME)  
OTHER CA INDEX NAMES:  
CN Benzenepropanoic acid, .beta.-amino-, methyl ester, (S)-  
OTHER NAMES:  
CN (S)-Methyl 3-amino-3-phenylpropanoate  
CN Methyl (3S)-3-amino-3-phenylpropionate  
FS STEREOSEARCH  
MF C10 H13 N O2  
CI COM  
LC STN Files: BEILSTEIN\*, CA, CAPLUS, CASREACT, CHEMINFORMRX, TOXCENTER, USPAT2, USPATFULL  
(\*File contains numerically searchable property data)  
DT.CA CAplus document type: Journal; Patent  
RL.P Roles from patents: PREP (Preparation); RACT (Reactant or reagent)  
RL.NP Roles from non-patents: PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent)

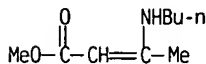
Absolute stereochemistry. Rotation (-).



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

44 REFERENCES IN FILE CA (1907 TO DATE)  
44 REFERENCES IN FILE CAPLUS (1907 TO DATE)

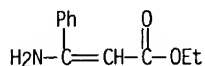
L5 ANSWER 19 OF 28 REGISTRY COPYRIGHT 2005 ACS on STN  
RN 36244-62-9 REGISTRY  
CN 2-Butenoic acid, 3-(butylamino)-, methyl ester (9CI) (CA INDEX NAME)  
OTHER NAMES:  
CN Methyl .beta.-(butylamino)crotonate  
CN Methyl 3-(butylamino)crotonic acid  
FS 3D CONCORD  
MF C9 H17 N O2  
LC STN Files: CA, CAPLUS, CASREACT, USPATFULL  
DT.CA CAplus document type: Journal; Patent  
RL.P Roles from patents: RACT (Reactant or reagent)  
RL.NP Roles from non-patents: PREP (Preparation); RACT (Reactant or reagent)



## \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

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4 REFERENCES IN FILE CAPLUS (1907 TO DATE)

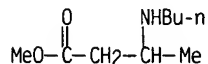
L5 ANSWER 20 OF 28 REGISTRY COPYRIGHT 2005 ACS on STN  
RN 33831-72-0 REGISTRY  
CN 2-Propenoic acid, 3-amino-3-phenyl-, ethyl ester (9CI) (CA INDEX NAME)  
OTHER CA INDEX NAMES:  
CN Cinnamic acid, .beta.-amino-, ethyl ester (6CI, 8CI)  
OTHER NAMES:  
CN Ethyl .beta.-aminocinnamate  
CN NSC 225260  
FS 3D CONCORD  
DR 291309-47-2  
MF C11 H13 N O2  
CI COM  
LC STN Files: BEILSTEIN\*, CA, CAOLD, CAPLUS, CASREACT, IFICDB, IFIPAT, IFIUIDB, TOXCENTER, USPATFULL  
(\*File contains numerically searchable property data)  
DT.CA CAplus document type: Journal; Patent  
RL.P Roles from patents: PREP (Preparation); RACT (Reactant or reagent); USES (Uses)  
RL.NP Roles from non-patents: PREP (Preparation); PROC (Process); RACT (Reactant or reagent); NORL (No role in record)



## \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

64 REFERENCES IN FILE CA (1907 TO DATE)  
64 REFERENCES IN FILE CAPLUS (1907 TO DATE)  
1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L5 ANSWER 21 OF 28 REGISTRY COPYRIGHT 2005 ACS on STN  
RN 14553-88-9 REGISTRY  
CN Butanoic acid, 3-(butylamino)-, methyl ester (9CI) (CA INDEX NAME)  
OTHER CA INDEX NAMES:  
CN Butyric acid, 3-(butylamino)-, methyl ester (8CI)  
FS 3D CONCORD  
MF C9 H19 N O2  
LC STN Files: BEILSTEIN\*, CA, CAPLUS, USPATFULL  
(\*File contains numerically searchable property data)  
DT.CA CAplus document type: Journal; Patent  
RL.P Roles from patents: PREP (Preparation)  
RL.NP Roles from non-patents: PREP (Preparation)

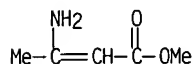


## \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

3 REFERENCES IN FILE CA (1907 TO DATE)  
3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L5 ANSWER 22 OF 28 REGISTRY COPYRIGHT 2005 ACS on STN  
RN 14205-39-1 REGISTRY

CN 2-Butenoic acid, 3-amino-, methyl ester (9CI) (CA INDEX NAME)  
 OTHER CA INDEX NAMES:  
 CN Crotonic acid, 3-amino-, methyl ester (7CI, 8CI)  
 OTHER NAMES:  
 CN .beta.-Aminocrotonic acid methyl ester  
 CN 3-Aminocrotonic acid methyl ester  
 CN Methyl .beta.-aminocrotonate  
 CN Methyl 3-amino-2-butenenoate  
 CN Methyl 3-amino-2-butenate  
 CN Methyl 3-aminocrotonate  
 CN Methyl 3-aminocrotonoate  
 FS 3D CONCORD  
 MF C5 H9 N O2  
 CI COM  
 LC STN Files: ANABSTR, BEILSTEIN\*, BIOBUSINESS, BIOSIS, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS, CHEMINFORMRX, CHEMLIST, CSCHEM, HODOC\*, IFICDB, IFIPAT, IFIADB, PS, RTECS\*, SPECINFO, SYNTHLINE, TOXCENTER, USPAT2, USPATFULL  
 (\*File contains numerically searchable property data)  
 Other Sources: DSL\*\*, EINECS\*\*, TSCA\*\*  
 (\*\*Enter CHEMLIST File for up-to-date regulatory information)  
 DT.CA CAPLUS document type: Journal; Patent  
 RL.P Roles from patents: ANST (Analytical study); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses); NORL (No role in record)  
 RL.NP Roles from non-patents: ANST (Analytical study); BIOL (Biological study); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent)  
 RLD.NP Roles for non-specific derivatives from non-patents: RACT (Reactant or reagent)



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

691 REFERENCES IN FILE CA (1907 TO DATE)  
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 691 REFERENCES IN FILE CAPLUS (1907 TO DATE)  
 1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

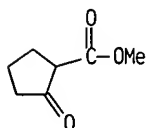
L5 ANSWER 23 OF 28 REGISTRY COPYRIGHT 2005 ACS on STN  
 RN 10472-24-9 REGISTRY  
 CN Cyclopentanecarboxylic acid, 2-oxo-, methyl ester (6CI, 8CI, 9CI) (CA INDEX NAME)  
 OTHER NAMES:  
 CN 2-(Methoxycarbonyl)cyclopentanone  
 CN 2-Carbomethoxycyclopentanone  
 CN 2-Oxocyclopentanecarboxylic acid methyl ester  
 CN Cyclopentenone-2-carboxylic acid methyl ester  
 CN Methyl 2-cyclopentanone-1-carboxylate  
 CN Methyl 2-oxo-1-cyclopentanecarboxylate  
 CN Methyl 2-oxocyclopentacarboxylate  
 CN Methyl 2-oxocyclopentanecarboxylate  
 FS 3D CONCORD  
 DR 53229-93-9  
 MF C7 H10 O3  
 CI COM  
 LC STN Files: BEILSTEIN\*, BIOBUSINESS, BIOSIS, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS, CHEMINFORMRX, CHEMLIST, CSCHEM, GMELIN\*, IFICDB, IFIPAT, IFIADB, SPECINFO, TOXCENTER, USPAT2, USPATFULL

(\*File contains numerically searchable property data)

Other Sources: EINECS\*\*, NDSL\*\*, TSCA\*\*

(\*\*Enter CHEMLIST File for up-to-date regulatory information)

DT.CA Caplus document type: Conference; Dissertation; Journal; Patent  
 RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); PROC (Process); RACT (Reactant or reagent); USES (Uses)  
 RL.NP Roles from non-patents: BIOL (Biological study); FORM (Formation, nonpreparative); OCCU (Occurrence); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses); NORL (No role in record)  
 RLD.NP Roles for non-specific derivatives from non-patents: FORM (Formation, nonpreparative); PROC (Process); PRP (Properties); RACT (Reactant or reagent)



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

407 REFERENCES IN FILE CA (1907 TO DATE)  
 2 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA  
 409 REFERENCES IN FILE CAPLUS (1907 TO DATE)  
 5 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L5 ANSWER 24 OF 28 REGISTRY COPYRIGHT 2005 ACS on STN

RN 3082-69-7 REGISTRY

CN Benzenepropanoic acid, .beta.-amino-, ethyl ester, (.beta.S)- (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN Benzenepropanoic acid, .beta.-amino-, ethyl ester, (S)-

CN Hydrocinnamic acid, .beta.-amino-, ethyl ester, (S)-(+)- (8CI)

OTHER NAMES:

CN (S)-Ethyl 3-amino-3-phenylpropionate

CN Ethyl (S)-3-amino-3-phenylpropanoate

FS STEREOSEARCH

MF C11 H15 N O2

CI COM

LC STN Files: BEILSTEIN\*, CA, CAOLD, CAPLUS, CASREACT, CHEMINFORMRX, TOXCENTER, USPAT2, USPATFULL

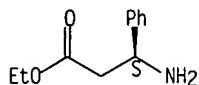
(\*File contains numerically searchable property data)

DT.CA Caplus document type: Journal; Patent

RL.P Roles from patents: PREP (Preparation); RACT (Reactant or reagent)

RL.NP Roles from non-patents: ANST (Analytical study); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); NORL (No role in record)

Absolute stereochemistry. Rotation (+).



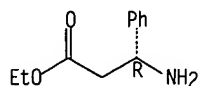
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18 REFERENCES IN FILE CA (1907 TO DATE)  
 18 REFERENCES IN FILE CAPLUS (1907 TO DATE)

## 1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L5 ANSWER 25 OF 28 REGISTRY COPYRIGHT 2005 ACS on STN  
 RN 3082-68-6 REGISTRY  
 CN Benzenepropanoic acid, .beta.-amino-, ethyl ester, (.beta.R)- (9CI) (CA INDEX NAME)  
 OTHER CA INDEX NAMES:  
 CN Benzenepropanoic acid, .beta.-amino-, ethyl ester, (R)-  
 CN Hydrocinnamic acid, .beta.-amino-, ethyl ester, (R)-(-)- (8CI)  
 FS STEREOSEARCH  
 MF C11 H15 N O2  
 CI COM  
 LC STN Files: BEILSTEIN\*, CA, CAOLD, CAPLUS, CASREACT, CHEMINFORMRX, USPATFULL  
 (\*File contains numerically searchable property data)  
 DT.CA CAplus document type: Journal; Patent  
 RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); PROC (Process)  
 RL.NP Roles from non-patents: ANST (Analytical study); BIOL (Biological study); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); NORL (No role in record)

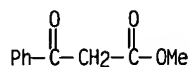
Absolute stereochemistry. Rotation (-).



## \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

10 REFERENCES IN FILE CA (1907 TO DATE)  
 10 REFERENCES IN FILE CAPLUS (1907 TO DATE)  
 1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

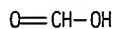
L5 ANSWER 26 OF 28 REGISTRY COPYRIGHT 2005 ACS on STN  
 RN 614-27-7 REGISTRY  
 CN Benzenepropanoic acid, .beta.-oxo-, methyl ester (9CI) (CA INDEX NAME)  
 OTHER CA INDEX NAMES:  
 CN Acetic acid, benzoyl-, methyl ester (6CI, 7CI, 8CI)  
 OTHER NAMES:  
 CN .beta.-Oxobenzenepropanoic acid methyl ester  
 CN 3-Oxo-3-phenylpropionic acid methyl ester  
 CN Methyl .beta.-oxobenzenepropanoate  
 CN Methyl 3-oxo-3-phenylpropanoate  
 CN Methyl 3-oxo-3-phenylpropionate  
 CN Methyl 3-phenyl-3-oxopropanoate  
 CN Methyl benzoylacetate  
 CN NSC 407764  
 FS 3D CONCORD  
 MF C10 H10 O3  
 LC STN Files: BEILSTEIN\*, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS, CHEMINFORMRX, CHEMLIST, CSCHEM, HODOC\*, IFICDB, IFIPAT, IFIUIDB, SPECINFO, TOXCENTER, USPATFULL  
 (\*File contains numerically searchable property data)  
 Other Sources: EINECS\*\*  
 (\*\*Enter CHEMLIST File for up-to-date regulatory information)  
 DT.CA CAplus document type: Journal; Patent  
 RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); PROC (Process); RACT (Reactant or reagent); USES (Uses)  
 RL.NP Roles from non-patents: BIOL (Biological study); FORM (Formation, nonpreparative); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); NORL (No role in record)



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

144 REFERENCES IN FILE CA (1907 TO DATE)  
 145 REFERENCES IN FILE CAPLUS (1907 TO DATE)  
 3 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L5 ANSWER 27 OF 28 REGISTRY COPYRIGHT 2005 ACS on STN  
 RN 540-69-2 REGISTRY  
 CN Formic acid, ammonium salt (8CI, 9CI) (CA INDEX NAME)  
 OTHER CA INDEX NAMES:  
 CN Ammonium formate (6CI)  
 DR 2787-68-0  
 MF C H2 O2 . H3 N  
 CI COM  
 LC STN Files: AGRICOLA, ANABSTR, BEILSTEIN\*, BIOBUSINESS, BIOSIS,  
 BIOTECHNO, CA, CABA, CAOLD, CAPLUS, CASREACT, CBNB, CEN, CHEMCATS,  
 CHEMINFORMRX, CHEMLIST, CIN, CSChem, DETHERM\*, EMBASE, GMELIN\*, HODOC\*,  
 HSDB\*, IFICDB, IFIPAT, IFIUDb, IPA, MRCK\*, MSDS-OHS, PDLCOM\*, PROMT, PS,  
 RTECS\*, SPECINFO, TOXCENTER, TULSA, USPAT2, USPATFULL  
 (\*File contains numerically searchable property data)  
 Other Sources: DSL\*\*, EINECS\*\*, TSCA\*\*  
 (\*\*Enter CHEMLIST File for up-to-date regulatory information)  
 DT.CA CAplus document type: Conference; Dissertation; Journal; Patent; Report  
 RL.P Roles from patents: ANST (Analytical study); BIOL (Biological study);  
 FORM (Formation, nonpreparative); MSC (Miscellaneous); OCCU  
 (Occurrence); PREP (Preparation); PROC (Process); PRP (Properties); RACT  
 (Reactant or reagent); USES (Uses); NORL (No role in record)  
 RLD.P Roles for non-specific derivatives from patents: BIOL (Biological  
 study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)  
 RL.NP Roles from non-patents: ANST (Analytical study); BIOL (Biological  
 study); FORM (Formation, nonpreparative); MSC (Miscellaneous); OCCU  
 (Occurrence); PREP (Preparation); PROC (Process); PRP (Properties); RACT  
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 CRN (64-18-6)

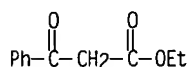


1184 REFERENCES IN FILE CA (1907 TO DATE)  
 12 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA  
 1189 REFERENCES IN FILE CAPLUS (1907 TO DATE)  
 32 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L5 ANSWER 28 OF 28 REGISTRY COPYRIGHT 2005 ACS on STN  
 RN 94-02-0 REGISTRY  
 CN Benzenepropanoic acid, .beta.-oxo-, ethyl ester (9CI) (CA INDEX NAME)  
 OTHER CA INDEX NAMES:  
 CN Acetic acid, benzoyl-, ethyl ester (6CI, 7CI, 8CI)

## OTHER NAMES:

CN .beta.-Oxobenzenepropanoic acid ethyl ester  
 CN 1-Ethoxy-3-phenylpropane-1,3-dione  
 CN 3-Oxo-3-phenylpropanoic acid ethyl ester  
 CN 3-Oxo-3-phenylpropionic acid ethyl ester  
 CN Benzoylacetic acid ethyl ester  
 CN Ethyl .beta.-oxobenzenepropanoate  
 CN Ethyl 2-benzoylacetate  
 CN Ethyl 3-oxo-3-phenylpropanoate  
 CN Ethyl 3-oxo-3-phenylpropionate  
 CN Ethyl 3-phenyl-3-oxopropanoate  
 CN Ethyl benzoylacetate  
 CN NSC 227214  
 CN NSC 6774  
 FS 3D CONCORD  
 MF C11 H12 O3  
 LC STN Files: AGRICOLA, BEILSTEIN\*, BIOBUSINESS, BIOSIS, CA, CAOLD, CAPLUS,  
 CASREACT, CHEMCATS, CHEMINFORMRX, CHEMLIST, CHEMSAFE, CSCHEM, DETHERM\*,  
 GMELIN\*, HODOC\*, IFICDB, IFIPAT, IFIUDB, MRCK\*, MSDS-OHS, RTECS\*,  
 SPECINFO, SYNTHLINE, TOXCENTER, USPAT2, USPATFULL  
 (\*File contains numerically searchable property data)  
 Other Sources: DSL\*\*, EINECS\*\*, TSCA\*\*  
 (\*\*Enter CHEMLIST File for up-to-date regulatory information)  
 DT.CA CAplus document type: Conference; Journal; Patent  
 RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); PROC  
 (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses);  
 NORL (No role in record)  
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 RACT (Reactant or reagent); USES (Uses); NORL (No role in record)  
 RLD.NP Roles for non-specific derivatives from non-patents: ANST (Analytical  
 study); PREP (Preparation); PRP (Properties); RACT (Reactant or reagent)



## \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

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 1925 REFERENCES IN FILE CAPLUS (1907 TO DATE)  
 41 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

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FILE 'WPIX' ENTERED AT 08:24:21 ON 23 FEB 2005  
 COPYRIGHT (C) 2005 THE THOMSON CORPORATION

FILE LAST UPDATED: 18 FEB 2005 <20050218/UP>  
 MOST RECENT DERWENT UPDATE: 200512 <200512/DW>  
 DERWENT WORLD PATENTS INDEX SUBSCRIBER FILE, COVERS 1963 TO DATE

>>> FOR A COPY OF THE DERWENT WORLD PATENTS INDEX STN USER GUIDE,  
 PLEASE VISIT:  
[http://www.stn-international.de/training\\_center/patents/stn\\_guide.pdf](http://www.stn-international.de/training_center/patents/stn_guide.pdf) <<<

>>> FOR DETAILS OF THE PATENTS COVERED IN CURRENT UPDATES, SEE  
<http://thomsonderwent.com/coverage/latestupdates/> <<<

>>> FOR INFORMATION ON ALL DERWENT WORLD PATENTS INDEX USER GUIDES, PLEASE VISIT:  
<http://thomsonderwent.com/support/userguides/> <<<

>>> NEW! FAST-ALERTING ACCESS TO NEWLY-PUBLISHED PATENT DOCUMENTATION NOW AVAILABLE IN DERWENT WORLD PATENTS INDEX FIRST VIEW - FILE WPIFV.  
 FOR FURTHER DETAILS: <http://www.thomsonderwent.com/dwpifv> <<<

>>> NEW DISPLAY FORMAT HITSTR ADDED ALLOWING DISPLAY OF HIT STRUCTURES WITHIN THE BIBLIOGRAPHIC DOCUMENT <<<

>>> SMILES and ISOSMILES strings are no longer available as Derwent Chemistry Resource display fields <<<

>>> THE CPI AND EPI MANUAL CODES HAVE BEEN REVISED FROM UPDATE 200501. PLEASE CHECK:  
<http://thomsonderwent.com/support/dwpieref/reftools/classification/code-revision/> FOR DETAILS. <<<

=> d all 18

L8 ANSWER 1 OF 1 WPIX COPYRIGHT 2005 THE THOMSON CORP on STN  
 AN 2004-204594 [20] WPIX  
 DNC C2004-080872  
 TI Production of an optically active beta-amino acid useful as intermediate for the production of, e.g. medicines, involves subjecting enamine to asymmetric hydrogenation.  
 DC B05 C03  
 IN MATSUMURA, K; SAITO, T; ZHANG, X  
 PA (TAKS) TAKASAGO INT CORP; (TAKS) TAKASAGO PERFUMERY CO LTD; (MATS-I) MATSUMURA K; (SAIT-I) SAITO T; (ZHAN-I) ZHANG X  
 CYC 33  
 PI EP 1386901 A1 20040204 (200420)\* EN 22 C07B053-00  
 R: AL AT BE BG CH CY CZ DE DK EE ES FI FR GB GR HU IE IT LI LT LU LV  
 MC MK NL PT RO SE SI SK TR  
 JP 2004075684 A 20040311 (200420) 27 C07C227-32  
 US 2004023344 A1 20040205 (200420) C12P013-04 <--  
 ADT EP 1386901 A1 EP 2003-16551 20030724; JP 2004075684 A JP 2003-282165 20030729; US 2004023344 A1 US 2003-628394 20030729  
 PRAI JP 2002-222149 20020730  
 IC ICM C07B053-00; C07C227-32; C12P013-04  
 ICS C07C229-08; C07C229-36; C07C303-32; C07C309-04  
 AB EP 1386901 A UPAB: 20040324  
 NOVELTY - Production of an optically active beta -amino acid involves subjecting an enamine to an asymmetric hydrogenation.  
 DETAILED DESCRIPTION - Production of an optically active beta -amino acid of formula (II) involves subjecting an enamine of formula (I) to an asymmetric hydrogenation.  
 b = 0 or 1;  
 the symbol asterisk = shows that the carbon atom is a chiral carbon;  
 R1 = H, alkyl, substituted alkyl, cycloalkyl, substituted cycloalkyl, aralkyl, substituted aralkyl, aryl, substituted aryl, aliphatic heterocyclic, substituted aliphatic heterocyclic, aromatic heterocyclic, substituted aromatic heterocyclic, alkoxy, substituted alkoxy, aralkyloxy, substituted aralkyloxy, aryloxy, or substituted aryloxy;  
 R2 = R1, alkyloxycarbonyl, or aralkyloxycarbonyl;  
 R3 = optionally substituted alkoxy, optionally substituted aralkyloxy, optionally substituted aryloxy, or optionally substituted amino group;  
 X' = acid;  
 R1 and R2, or R2 and R3 = may be combined together to form a ring;

a = 0 or 1.

R1 and R2 are not H simultaneously.

USE - The method is used for producing an optically active beta-amino acid useful as intermediate for the production of medicines, agricultural chemicals, and physiologically active substances, particularly as intermediate for the synthesis of antibiotics.

ADVANTAGE - The inventive method is of high performance and high enantiomeric excess, and does not require additional procedures, e.g. introduction and removal of protecting group. It provides optically active beta-amino acid of excellent optical purity with small amount of catalyst and in a short process without undergoing, e.g. deprotection.

Dwg.0/0

FS CPI

FA AB; GI; DCN

MC CPI: B10-B02B; C10-B02B

=> b home

FILE 'HOME' ENTERED AT 08:24:37 ON 23 FEB 2005

=>

=&gt; d his

(FILE 'HOME' ENTERED AT 08:21:41 ON 23 FEB 2005)

FILE 'HCAPLUS' ENTERED AT 08:21:51 ON 23 FEB 2005

L1 1 US20040023344/PN  
E JP2002-222149/AP,PRN  
L2 1 JP2002-222149/AP,PRN  
L3 1 L1-2

FILE 'REGISTRY' ENTERED AT 08:22:32 ON 23 FEB 2005

FILE 'HCAPLUS' ENTERED AT 08:22:34 ON 23 FEB 2005  
L4 TRA L3 1- RN : 28 TERMS

FILE 'REGISTRY' ENTERED AT 08:22:34 ON 23 FEB 2005  
L5 28 SEA L4

FILE 'WPIX' ENTERED AT 08:22:37 ON 23 FEB 2005

L6 1 US20040023344/PN  
E JP2002-222149/AP,PRN  
L7 1 JP2002-222149/AP,PRN  
L8 1 L6-7

FILE 'CASREACT' ENTERED AT 08:42:17 ON 23 FEB 2005

L9 STR  
L10 0 L9  
L11 SCR 2039 OR 2050 OR 2049 OR 2048 OR 2053 OR 2052 OR 2043 OR 205  
L12 STR L9  
L13 0 L12 NOT L11 CSS  
L14 STR L12  
L15 1 L14 NOT L11 CSS  
L16 30 L14 NOT L11 CSS FULL  
SAV TEM SHIAO394F0/A L16  
E MATSUMURA K/AU  
L17 16 E6  
E ZHANG X/AU  
L18 36 E3-12  
E ZHANG XIAOYONG/AU  
L19 7 E3  
E SAITO T/AU  
L20 89 E3,E11  
L21 106 (TAKASAGO (1A) INT? (1A) CORP?)/CS,PA  
L22 0 L16 AND L17-21  
L23 QUE PY<=2002 OR AY<=2002 OR PRY<=2002 OR PD<20020730 OR AD<2002  
L24 28 L16 AND L23

=&gt; b casre

FILE 'CASREACT' ENTERED AT 09:05:47 ON 23 FEB 2005  
USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT  
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FILE CONTENT:1840 - 20 Feb 2005 VOL 142 ISS 8

\*\*\*\*\*  
\* CASREACT now has more than 8 million reactions \*  
\*  
\*\*\*\*\*

Some CASREACT records are derived from the ZIC/VINITI database (1974-1991) provided by InfoChem, INPI data prior to 1986, and Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance identification.

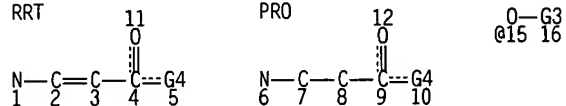
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L11 SCR 2039 OR 2050 OR 2049 OR 2048 OR 2053 OR 2052 OR 2043 O

R 2054

L14 STR

RRT PRO O-G3 N@17



VAR G3=AK/CY

VAR G4=15/17

NODE ATTRIBUTES:

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CONNECT IS M1 RC AT 2

CONNECT IS M1 RC AT 3

CONNECT IS M1 RC AT 7

CONNECT IS M1 RC AT 8

CONNECT IS M1 RC AT 17

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 15

STEREO ATTRIBUTES: NONE

L16 30 SEA FILE=CASREACT CSS FUL L14 NOT L11 ( 82 REACTIONS)

100.0% DONE 4411 VERIFIED 82 HIT RXNS 30 DOCS

SEARCH TIME: 00.00.01

=> d bib abs ind retable crd 124 tot

L24 ANSWER 1 OF 28 CASREACT COPYRIGHT 2005 ACS on STN

AN 138:338002 CASREACT

TI Reaction of 3-Cyano-2-amino-4,5,6,7-tetrahydrobenzo[b]thiophene with Enamino nitriles

AU Mohareb, Rafat M.; Al-Omran, Fatma A.; Ho, Jonathan Z.

CS Department of Chemistry, University of California, Berkeley, CA, 94720, USA

SO Monatshefte fuer Chemie (2002), 133(11), 1443-1452

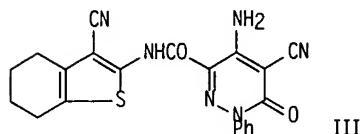
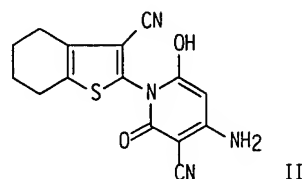
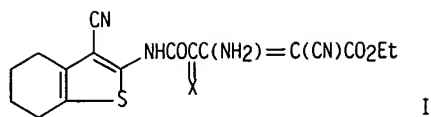
CODEN: MOCMB7; ISSN: 0026-9247

PB Springer-Verlag Wien

DT Journal

LA English

GI



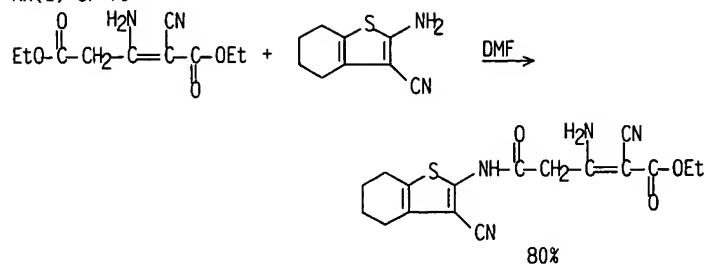
- AB 2-Amino-3-cyano-4,5,6,7-tetrahydrobenzo[b]thiophene with Et .beta.-amino-.alpha.-cyano-.gamma.-(ethoxycarbonyl)crotonate yields the corresponding amide derivative (I, X = H<sub>2</sub>). That compound reacts with benzenediazonium chloride to give the phenylhydrazone derivative (I, X = NNHPh). These compds. were cyclized to give a pyridine derivative (II) and a pyridazine derivative (III). Reactions of II gave fused heterocyclic compds. with antibacterial activity.
- CC 28-1 (Heterocyclic Compounds (More Than One Hetero Atom))  
Section cross-reference(s): 1
- ST benzothiophenecarbonitrile aminotetrahydro reaction enamino nitrile;  
pyridine fused deriv prepn antibacterial activity; pyridazine deriv prepn  
antibacterial activity
- IT Antibacterial agents  
Heterocyclization  
(reaction of 2-amino-3-cyano-4,5,6,7-tetrahydrobenzo[b]thiophene with enamino nitrile, heterocyclization reactions, and antibacterial activity of the products)
- IT 62-56-6, Thiourea, reactions 7357-70-2, Cyanothioacetamide  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(heterocyclization reaction with bromohydroxypyridinone derivative)
- IT 90-02-8, Salicylaldehyde, reactions 2025-40-3, Ethyl  
benzylidenecyanoacetate 2700-22-3, Benzylidenemalononitrile  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(heterocyclization reaction with thiazolopyridineacetonitrile derivative)
- IT 515876-52-5P 515876-54-7P  
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)  
(intermediate; reaction of 2-amino-3-cyano-4,5,6,7-tetrahydrobenzo[b]thiophene with enamino nitrile, heterocyclization reactions, and antibacterial activity of the products)
- IT 515876-37-6P 515876-39-8P 515876-45-6P 515876-47-8P 515876-48-9P  
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)  
(reaction of 2-amino-3-cyano-4,5,6,7-tetrahydrobenzo[b]thiophene with enamino nitrile, heterocyclization reactions, and antibacterial activity of the products)
- IT 515876-38-7P 515876-40-1P 515876-44-5P 515876-46-7P 515876-49-0P  
515876-50-3P 515876-51-4P 515876-55-8P 515876-56-9P  
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

- (reaction of 2-amino-3-cyano-4,5,6,7-tetrahydrobenzo[b]thiophene with enamino nitrile, heterocyclization reactions, and antibacterial activity of the products)
- IT 4651-91-6 28447-79-2  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of 2-amino-3-cyano-4,5,6,7-tetrahydrobenzo[b]thiophene with enamino nitrile, heterocyclization reactions, and antibacterial activity of the products)
- IT 515876-36-5P 515876-41-2P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(reaction of 2-amino-3-cyano-4,5,6,7-tetrahydrobenzo[b]thiophene with enamino nitrile, heterocyclization reactions, and antibacterial activity of the products)
- IT 515876-42-3P 515876-43-4P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(reaction of 2-amino-3-cyano-4,5,6,7-tetrahydrobenzo[b]thiophene with enamino nitrile, heterocyclization reactions, and antibacterial activity of the products)
- IT 109-77-3, Malononitrile  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction with aminobenzylidenecyano(ethoxycarbonyl)butenamide derivative)
- IT 105-56-6, Ethyl cyanoacetate  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction with aminocyano(cyanobenzo[b]thienyl)hydroxypyridinone)
- IT 100-34-5, Benzenediazonium chloride 100-52-7, Benzaldehyde, reactions  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction with aminocyano(ethoxycarbonyl)butenamide derivative)
- IT 100-63-0, Phenylhydrazine 302-01-2, Hydrazine, reactions  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction with aminocyano(ethoxycarbonyl)butenamide derivative)

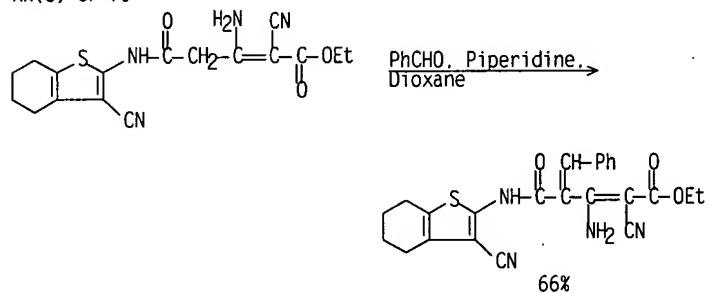
## RETABLE

Referenced Author (RAU)	Year (RPY)	VOL (RVL)	PG (RPG)	Referenced Work (RWK)	Referenced File
Amidshiro, S	1999	42	669	J Med Chem	
Bakonyi, M	1998	51	681	PCT Int Appl Wo	CAPLUS
Baraldi, G	1999	21	617	PCT Int Appl Wo	CAPLUS
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El-Feky, S	1995	50	341	Pharmazie	CAPLUS
Fahmy, S	1984	11	976	Synthesis	
Fujii, K	1999			JP 11116555	CAPLUS
Gutter, Y	1982	89	332	Pflanzenker Pflanzen	CAPLUS
Mohareb, R	2000	11	403	Heteroat Chem	CAPLUS
Mohareb, R	2001	12	168	Heteroat Chem	CAPLUS
Mohareb, R	2001	12	518	Heteroat Chem	CAPLUS
Nanteuil, G	1995	45	1175	Arzneim-Forsch/Drug	
Sadek, K	1984	29	101	J Chem Engin Data	CAPLUS
Schachtner, E	1998	33	665	Eu J Med Chem	
Schafer, P	1999			WO 19990325	CAPLUS
Shachnai, Y	1981	189	64	Bull Merkaz Volcani	CAPLUS
Wolfbeis, O	1981	112	875	Monatsh Fur Chem	CAPLUS

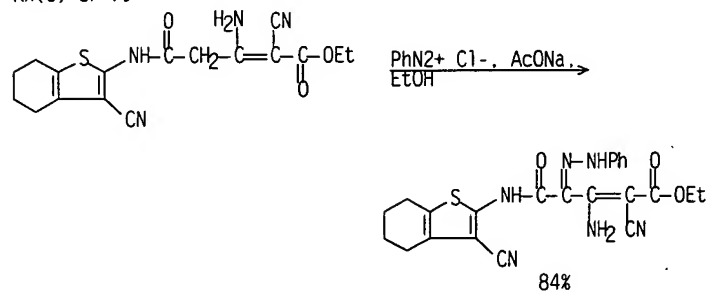
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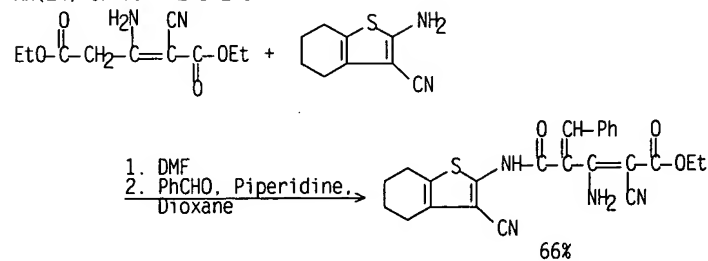
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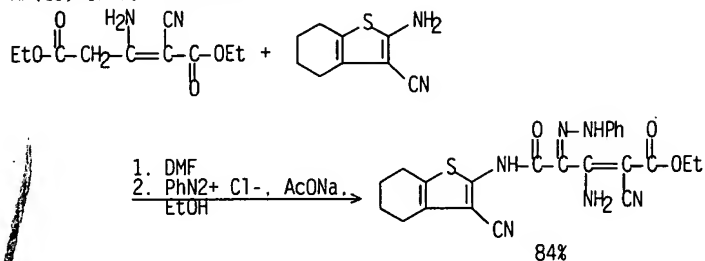
RX(6) OF 79



RX(24) OF 79 - 2 STEPS



RX(25) OF 79 - 2 STEPS



L24 ANSWER 2 OF 28 CASREACT COPYRIGHT 2005 ACS on STN

AN 138:221836 CASREACT

TI Process for preparation of enantiomerically enriched beta-amino acid intermediate for synthesis of chiral integrin antagonists

IN Rivera, Nelo R.; Welch, Christopher J.; Xiao, Yi; Yasuda, Nobuyoshi

PA Merck &amp; Co., Inc., USA

SO U.S. Pat. Appl. Publ., 8 pp.

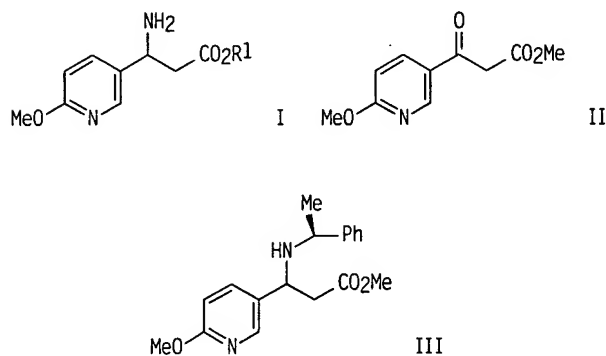
CODEN: USXXCO

DT Patent

LA English

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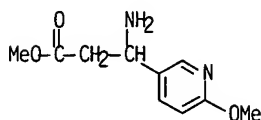
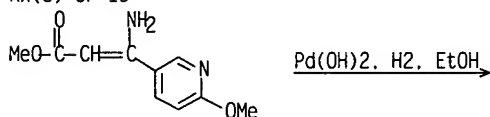
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	US 6646130	B2	20031111		
PRAI	US 2001-306502P		20010719		
OS	MARPAT 138:221836				
GI					



AB This invention discloses a novel process for the preparation of enantiomerically enriched mixts. of compds. I (R<sub>1</sub> = C<sub>1</sub>-4 alkyl) which are useful intermediates in the synthesis of  $\alpha$ .v. $\beta$ .3 integrin receptor antagonists. Thus, condensation of keto ester II (preparation given) with (S)-(-)-1-phenylethylamine gave the corresponding enamine, which underwent hydrogenation in 10% AcOH/MeOH in the presence of PtO<sub>2</sub> for 15 h. to give a 3:1 mixture of diastereomers III. Hydrogenolysis of III in 10% AcOH/MeOH in the presence of Pd(OH)<sub>2</sub> gave enantiomerically enriched ester I (R = Me) as the acetate salt. Resolution of enantiomerically enriched I (R = Me) was carried out by crystallization with N-benzoyloxycarbonyl-(S)-phenylalanine. The recovered crystalline salt had an enantiomeric excess of 98% as determined by chiral HPLC.

IC ICM A61K031-44  
ICS C07D213-78  
NCL 514351000  
CC 34-2 (Amino Acids, Peptides, and Proteins)  
ST beta amino acid integrin antagonist intermediate asym synthesis: crystn  
purifn protected amino acid beta amino acid  
IT Amino acids, reactions  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(N-protected; purification of .beta.-amino acid intermediate via crystallization  
with N-protected amino acids)  
IT Asymmetric synthesis and induction  
(process for preparation of enantiomerically enriched .beta.-amino acid  
intermediate for synthesis of chiral integrin antagonists)  
IT Crystallization  
(purification of .beta.-amino acid intermediate via crystallization with N-protected  
amino acids)  
IT 500795-51-7P 500795-56-2P 500795-57-3P  
RL: PUR (Purification or recovery); RCT (Reactant); SPN (Synthetic  
preparation); PREP (Preparation); RACT (Reactant or reagent)  
(process for preparation of enantiomerically enriched .beta.-amino acid  
intermediate for synthesis of chiral integrin antagonists)  
IT 1161-13-3, N-Benzyloxycarbonyl-(S)-phenylalanine 2627-86-3,  
(S)-1-Phenylethylamine 38330-80-2, Potassium monomethylmalonate  
66572-55-2, 6-Methoxynicotinic acid  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(process for preparation of enantiomerically enriched .beta.-amino acid  
intermediate for synthesis of chiral integrin antagonists)  
IT 500795-49-3P 500795-50-6P 500795-54-0P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)  
(process for preparation of enantiomerically enriched .beta.-amino acid  
intermediate for synthesis of chiral integrin antagonists)  
IT 500795-53-9P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(process for preparation of enantiomerically enriched .beta.-amino acid  
intermediate for synthesis of chiral integrin antagonists)

RX(3) OF 15



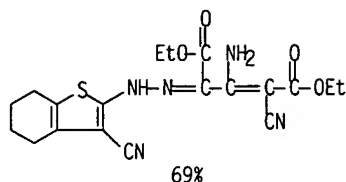
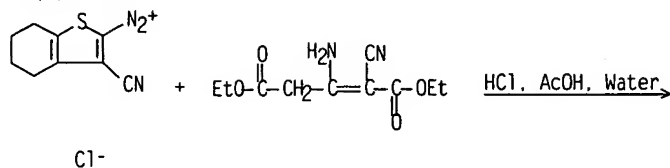
L24 ANSWER 3 OF 28 CASREACT COPYRIGHT 2005 ACS on STN  
AN 137:169474 CASREACT  
TI Uses of 2-diazo-4,5,6,7-tetrahydrobenzo[b]thiophene derivatives in the  
synthesis of azoles, azines, and their fused derivatives  
AU Wardakhan, Wagnat W.; Fleita, Daisy H.  
CS Department of Chemistry, University of California, Berkeley, CA, 94720,  
USA  
SO Heteroatom Chemistry (2002), 13(2), 108-115  
CODEN: HETCE8; ISSN: 1042-7163  
PB John Wiley & Sons, Inc.  
DT Journal  
LA English

- AB The reactions of 2-diazo-4,5,6,7-tetrahydrobenzo[b]thiophene derivs. with RCH<sub>2</sub>C(NH<sub>2</sub>):CRCN [R = CO<sub>2</sub>Et, CN] gave the hydrazone derivs. The reactivity of the latter products towards various chemical reagents was studied in order to provide azole and azine derivs. incorporating the thiophene ring, and most of them showed high antimicrobial activity.
- CC 28-15 (Heterocyclic Compounds (More Than One Hetero Atom))  
Section cross-reference(s): 10
- ST bactericide pyridazinone pyridotriazinethione pyrazolopyridine pyridazinopyrimidine benzothienyl prepn; benzothienopyridazinopyrimidinone prepn bactericide
- IT Antibacterial agents  
(preparation of bactericidal azoles, azines, and their fused derivs. from 2-diazo-4,5,6,7-tetrahydrobenzo[b]thiophene derivs.)
- IT 446253-83-4P 446253-84-5P 446253-87-8P 446253-88-9P 446253-90-3P  
446253-92-5P 446253-94-7P 446253-96-9P  
RL: BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)  
(preparation of bactericidal azoles, azines, and their fused derivs. from 2-diazo-4,5,6,7-tetrahydrobenzo[b]thiophene derivs.)
- IT 446253-85-6P 446253-86-7P 446253-89-0P 446253-91-4P 446253-93-6P  
446253-95-8P 446253-97-0P 446253-98-1P  
RL: BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)  
(preparation of bactericidal azoles, azines, and their fused derivs. from 2-diazo-4,5,6,7-tetrahydrobenzo[b]thiophene derivs.)
- IT 98-86-2, Acetophenone, reactions 105-56-6, Ethyl cyanoacetate 109-77-3, Malononitrile 868-54-2 2700-22-3, Benzylidenemalononitrile 28447-79-2 446253-82-3  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(preparation of bactericidal azoles, azines, and their fused derivs. from 2-diazo-4,5,6,7-tetrahydrobenzo[b]thiophene derivs.)

## RETABLE

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Clark, J	1984		2005	J Chem Soc Perkin Tr	CAPLUS
El-Dean, A	1998	129	523	Monatsh Chem	CAPLUS
El-Feky, S	1995	50	341	Pharmazie	CAPLUS
Geies, A	1998		1248	J Chem Res Miniprint	
Geies, A	1998		290	J Chem Res Synop	CAPLUS
Gutter, Y	1982	89	332	Pflanzenkr Pflanzenu	CAPLUS
Gutter, Y	1982	97	143345	Z Chem Abstr	
Hozien, Z	1996	26	3733	Synth Commun	CAPLUS
Magni, A	1994	44	1420	Arzneim-Forsch, J D	
Meeson, M	1995	38	2763	J Med Chem	
Mohareb, R	2001	12	168	Heteroat Chem	CAPLUS
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Shishoo, C	1990	40	567	Arzneim-Forsch	CAPLUS
Taylor, E	1996	43	349	Heterocycles	CAPLUS
Wardakhan, W	2000	162	275	Phosphorus Sulfur Si	CAPLUS
Zodi, H	1996		2526	J Chem Res Miniprint	
Zodi, H	1996		440	J Chem Res Synop	

RX(2) OF 39



L24 ANSWER 4 OF 28 CASREACT COPYRIGHT 2005 ACS on STN

AN 135:344327 CASREACT

TI [2+2] Cycloaddition reactions of 1-benzyl-2,4-diphenyl-1,3-diazabuta-1,3-diene with chiral ketenes

AU Abbiati, G.; Rossi, E.

CS Istituto di Chimica Organica della Facolta di Farmacia, Universita di Milano, Milan, I-20133, Italy

SO Tetrahedron (2001), 57(33), 7205-7212

CODEN: TETRAB; ISSN: 0040-4020

PB Elsevier Science Ltd.

DT Journal

LA English

AB The [2+2] cycloaddn. reactions of 1-benzyl-2,4-diphenyl-1,3-diaza-1,3-butadiene [i.e., N'-(phenylmethyl)-N-(phenylmethylene)benzenecarboximidamide] with .beta.-(dimethylphenylsilyl)ketene, .beta.-menthoxyketene and Evans-Sjogren ketene were investigated. The results and some chemical transformations of the obtained cycloadducts are reported.

CC 27-5 (Heterocyclic Compounds (One Hetero Atom))

ST chiral ketene cycloaddn diazabutadiene; ethenone chiral cycloaddn diazabutadiene; benzenecarboximidamide phenylmethylene cycloaddn ketene; azetidinone phenylmethylenamino prepn

IT Cycloaddition reaction

([2+2]: [2+2] cycloaddn. of 1-benzyl-2,4-diphenyl-1,3-diazabuta-1,3-diene with chiral ketenes)

IT 525-06-4, Diphenylketene 598-26-5, Dimethylketene 3496-32-0, Phenylketene 4591-28-0, Dichloroketene 29804-89-5, Chloroketene 35848-87-4 50888-73-8, Vinylketene 54276-52-7, Methoxyketene 73786-06-8, Azidoketene 108493-67-0 120346-31-8 371961-63-6 371961-64-7

RL: RCT (Reactant); RACT (Reactant or reagent)

([2+2] cycloaddn. of 1-benzyl-2,4-diphenyl-1,3-diazabuta-1,3-diene with chiral ketenes)

IT 371961-65-8P 371961-70-5P 371961-71-6P 371961-73-8P 371961-76-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation of)

IT 5100-01-6P 198630-86-3P 233257-71-1P 233257-72-2P 233257-73-3P  
233257-74-4P 233257-75-5P 233257-76-6P 371961-66-9P 371961-67-0P  
371961-68-1P 371961-69-2P 371961-72-7P 371961-74-9P 371961-78-3P  
371961-79-4P 371961-81-8P 371961-82-9P

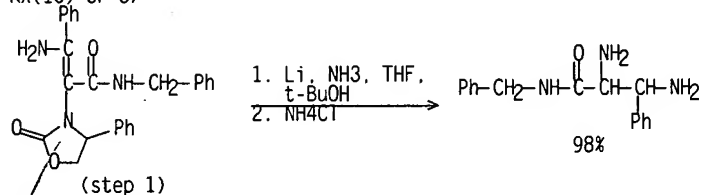
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RETABLE

Referenced Author	Year	VOL	PG	Referenced Work	Referenced
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Boger, D	1991	56	5385	J Org Chem	CAPLUS
Bose, A	1982	47	4075	J Org Chem	CAPLUS
Buckle, M	1992	33	4479	Tetrahedron Lett	CAPLUS
Burwood, M	1995	36	9053	Tetrahedron Lett	CAPLUS
Dewar, M	1985	107	3902	J Am Chem Soc	CAPLUS
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Durkheimer, W	1985	97	183	Angew Chem, Int Ed E	
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Fleming, I	1984		1805	J Chem Soc, Perkin T	CAPLUS
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Ishibashi, H	1995	60	1276	J Org Chem	CAPLUS
Kidwai, M	1999	6	195	Curr Med Chem	CAPLUS
Knouzi, N	1985	5	815	Bull Soc Chim Fr	
Leffler, M	1955		547	Organic Synthesis Co	
Mascaretti, O	1995	1	441	Curr Med Chem	CAPLUS
Morin, R	1982	1-3		Chemistry and Biolog	
Narasimhan, N	1965	46	4145	Tetrahedron Lett	
Ojima, I	1990	112	770	J Am Chem Soc	CAPLUS
Ojima, I	1990	31	977	Tetrahedron Lett	CAPLUS
Ojima, I	1993			The Organic Chemistr	
Ojima, J	1995	28	383	Acc Chem Res	
Palomo, C	1999		3223	Eur J Org Chem	CAPLUS
Palomo, C	1994	59	240	J Org Chem	CAPLUS
Palomo, C	1997	62	2070	J Org Chem	CAPLUS
Ram, S	1987	28	515	Tetrahedron Lett	CAPLUS
Rossi, E	1997	53	14107	Tetrahedron	CAPLUS
Rossi, E	1999	55	6961	Tetrahedron	
Southgate, R	1994	1	417	Contemp Org Synth	CAPLUS
Southgate, R	1993	2	621	Progress in the Chem	
Southgate, R	1985	47		The Chemistry of Org	CAPLUS
Staudinger, H	1907	356	51	Liebigs Ann Chem	CAPLUS
Sudarsanam, V	1982	21B	989	Indian J Chem	CAPLUS

RX(16) OF 37



L24 ANSWER 5 OF 28 CASREACT COPYRIGHT 2005 ACS on STN

AN 135:195787 CASREACT

TI Method of producing 3-aminoalkanoic acid esters via catalytic hydrogenation of 3-amino-2-alkenoic acid esters

IN Fuchs, Rudolf

PA Lonza A.-G., Switz.

SO PCT Int. Appl.. 14 pp.

CODEN: PIXXD2

DT Patent

LA German

FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001062707	A1	20010830	WO 2001-EP1955	20010221

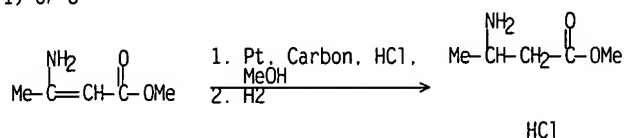
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 RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG  
 EP 1257523 A1 20021120 EP 2001-911673 20010221  
 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR  
 JP 2003523990 T2 20030812 JP 2001-561717 20010221  
 US 2003114704 A1 20030619 US 2002-204461 20020821  
 US 6784311 B2 20040831  
 PRAI EP 2000-103714 20000222  
 US 2000-203902P 20000512  
 WO 2001-EP1955 20010221  
 OS MARPAT 135:195787  
 AB The invention relates to a method of producing 3-aminoalkanoic acid esters RICH(NH<sub>2</sub>)CH<sub>2</sub>C(O)OR [(I); R = alkyl; R<sub>1</sub> = H, alkyl or Ph] or the salts thereof, by catalytic hydrogenation of corresponding 3-amino-2-alkenoic acid esters in the presence of a strong acid. Thus, 5 g Me 3-amino-2-butenate, HCl gas in water-free MeOH, and Pt/C catalyst were mixed at 21-25.degree. and 5-10 bar H<sub>2</sub> pressure for 3 h., the catalyst filtered, and the racemic HCl salt product I [R, R<sub>1</sub> = Me] purified (yield 6.34 g). Similarly prepared were sulfate and methanesulfonate salts of Me (RS)-3-aminobutanoate.  
 IC ICM C07C227-14  
 CC 34-2 (Amino Acids, Peptides, and Proteins)  
 ST catalytic hydrogenation aminoalkenoate prepn amino alkanoate salt  
 IT Hydrogenation  
 Hydrogenation catalysts  
 (preparation of .beta.-amino acid ester salts via catalytic hydrogenation of 3-amino-2-alkenoic acid esters)  
 IT Esters, preparation  
 Salts, preparation  
 RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation of .beta.-amino acid ester salts via catalytic hydrogenation of 3-amino-2-alkenoic acid esters)  
 IT Amino acids, preparation  
 RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)  
 (.beta.-: preparation of .beta.-amino acid ester salts via catalytic hydrogenation of 3-amino-2-alkenoic acid esters)  
 IT 7440-44-0, Carbon, uses  
 RL: CAT (Catalyst use); USES (Uses)  
 (activated; preparation of .beta.-amino acid ester salts via catalytic hydrogenation of 3-amino-2-alkenoic acid esters)  
 IT 7440-05-3D, Palladium, catalysts, uses 7440-06-4D, Platinum, catalysts, uses 7440-16-6D, Rhodium, catalysts, uses  
 RL: CAT (Catalyst use); USES (Uses)  
 (preparation of .beta.-amino acid ester salts via catalytic hydrogenation of 3-amino-2-alkenoic acid esters)  
 IT 137132-12-8P 356039-97-9P 356039-98-0P  
 RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of .beta.-amino acid ester salts via catalytic hydrogenation of 3-amino-2-alkenoic acid esters)  
 IT 75-75-2, Methanesulfonic acid 76-05-1, Trifluoroacetic acid, reactions 104-15-4, p-Toluenesulfonic acid, reactions 7647-01-0, Hydrogen chloride, reactions 7664-93-9, Sulfuric acid, reactions 14205-39-1, 3-Aminocrotonic acid, methyl ester

RL: RCT (Reactant); RACT (Reactant or reagent)  
(preparation of .beta.-amino acid ester salts via catalytic hydrogenation of  
3-amino-2-alkenoic acid esters)

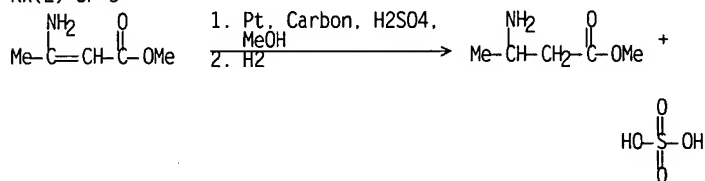
## RETABLE

Referenced Author (RAU)	Year (RPY)	VOL (RVL)	PG (RPG)	Referenced Work (RWK)	Referenced File
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Bartoli	1994	59	5328	J ORG CHEM	CAPLUS
Lonza Ag	1985			EP 0144980 A	CAPLUS
Murzagulova, K					CAPLUS
Murzagulova, K	1998	32	52	KHIM -FARM ZH	CAPLUS

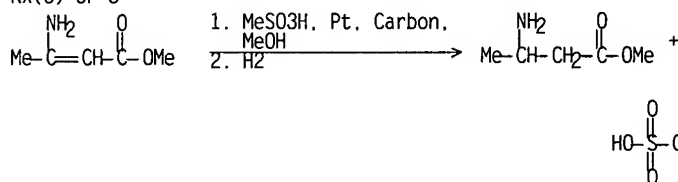
## RX(1) OF 3



## RX(2) OF 3



## RX(3) OF 3



L24 ANSWER 6 OF 28 CASREACT COPYRIGHT 2005 ACS on STN

AN 135:152620 CASREACT

TI Method for producing acetoacetylated aromatic amines

IN Glufke, Uta; Hanselmann, Paul

PA Lonza A.-G., Switz.

SO PCT Int. Appl.. 19 pp.

CODEN: PIXXD2

DT Patent

LA German

FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2001056973	A1	20010809	WO 2001-EP1163	20010202

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, US, US

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,  
 DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF,  
 BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

AU 2001039239	A5	20010814	AU 2001-39239	20010202
EP 1252134	A1	20021030	EP 2001-913783	20010202
EP 1252134	B1	20041006		

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,  
 IE, SI, LT, LV, FI, RO, MK, CY, AL, TR

AT 278660	E	20041015	AT 2001-913783	20010202
EP 1496047	A1	20050112	EP 2004-21980	20010202

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,  
 IE, FI, CY, TR

US 2003125392	A1	20030703	US 2002-182916	20021021
US 6734324	B2	20040511		
US <del>2004152919</del>	A1	20040805	US 2004-761399	20040122

PRAI EP 2000-102418 20000204  
 US 2000-203922P 20000512  
 EP 2001-913783 20010202  
 WO 2001-EP1163 20010202  
 US 2002-182916 20021021

OS MARPAT 135:152620  
 GI

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB The invention relates to a method for producing acetoacetylated aromatic amines I [R1 and R2, each time they occur and independently of each other, mean hydroxy, C1-6-alkyl, C1-6-alkoxy, halogen, Ph or phenoxy; R3 means hydrogen or C1-6-alkyl; m is a whole number from 0 to 4; and n is a whole number from 0 to 5]. According to said method, diketene is reacted with a N-phenyl-p-phenylenediamine derivs. II [R1, R2, R3, m and n have the meanings given above], in the presence of 3-40% acetic acid and at temps. of 20 to 100 .degree.C, preferably 60 to 70 .degree.C. The invention also relates to the compds. I [R3 = C1-6-alkyl] and the enamines III that can be obtained from these by reaction with ammonia, and their hydrogenation products IV.

IC ICM C07C231-04  
 ICS C07C237-16; C07C237-10; C07C231-12

CC 25-4 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)  
 Section cross-reference(s): 23

ST arom amine acetoacetylation; diketene condensation phenylenediamine deriv;  
 enamine acetoacetamide prepn hydrogenation; aminobutyramide prepn

IT Acetylation  
 (acetoacetylation; preparation of acetoacetylated aromatic amines via condensation of diketene with N-phenyl-p-phenylenediamine derivs.)

IT Amines, preparation  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (aromatic; preparation of acetoacetylated aromatic amines via condensation of diketene with N-phenyl-p-phenylenediamine derivs.)

IT Hydrogenation  
 (preparation of acetoacetylated aromatic amines via condensation of diketene with N-phenyl-p-phenylenediamine derivs.)

IT Enamines  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation of acetoacetylated aromatic amines via condensation of diketene with N-phenyl-p-phenylenediamine derivs.)

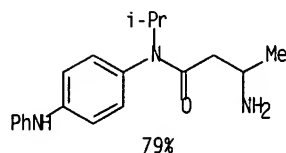
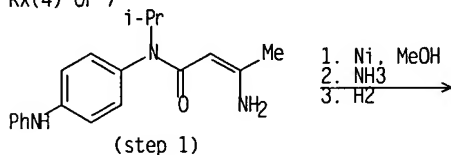
IT 347895-01-6P 353236-69-8P  
 RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

- (preparation of acetoacetylated aromatic amines via condensation of diketene with N-phenyl-p-phenylenediamine derivs.)
- IT 38971-14-1P 347895-03-8P  
 RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of acetoacetylated aromatic amines via condensation of diketene with N-phenyl-p-phenylenediamine derivs.)
- IT 64-19-7, Acetic acid, uses  
 RL: NUU (Other use, unclassified); USES (Uses)  
 (preparation of acetoacetylated aromatic amines via condensation of diketene with N-phenyl-p-phenylenediamine derivs.)
- IT 101-54-2, N-Phenyl-p-phenylenediamine 101-54-2D, N-Phenyl-p-phenylenediamine, derivs. 674-82-8, Diketene 3085-82-3, N-Isopropyl-N-phenyl-p-phenylenediamine 7664-41-7, Ammonia, reactions  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (preparation of acetoacetylated aromatic amines via condensation of diketene with N-phenyl-p-phenylenediamine derivs.)

## RETABLE

Referenced Author (RAU)	Year (RPY)	VOL (RVL)	PG (RPG)	Referenced Work (RWK)	Referenced File
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Chevron Chem Co	1996			EP 0719762 A	CAPLUS
Deutsche Gold- Und Silb	1968			ZA 67068521	CAPLUS
Thiele, K	1972			US 3702365 A	CAPLUS

RX(4) OF 7



NOTE: Raney nickel

103 (9)

- L24 ANSWER 7 OF 28 CASREACT COPYRIGHT 2005 ACS on STN
- AN 134:71479 CASREACT
- TI Synthesis and antiproliferative activity of unsaturated quinoline derivatives
- AU Montgomery, Gerard J.; McKeown, Paul; McGown, Alan T.; Robins, David J.
- CS Department of Chemistry, University of Glasgow, Glasgow, G12 8QQ, UK
- SO Anti-Cancer Drug Design (2000), 15(3), 171-181  
 CODEN: ACDDDEA; ISSN: 0266-9536
- PB Oxford University Press
- DT Journal
- LA English
- AB Knoevenagel condensation of quinoline 6-, 7- and 8-carboxaldehyde with malononitrile derivs. was used to produce a series of 23 quinoline-tyrphostins. Some of these heteroarom. tyrphostins were potent inhibitors of the epidermal growth factor (EGF) receptor kinase and were moderately active against the MCF7 breast cancer cell line. The order of potency was 7- > 6- > 8-substituted quinoline, which indicates that increased activity of the 7-substituted quinolines is associated with electron deficiency at the 7-position in the quinoline ring. The most active compound, formed from 7-quinolinecarboxaldehyde and Et cyanoacetate,

had an IC50 value of 2.3  $\mu$ M. The prepared compds. showed similar IC50 values against the MCF7 and MCF7/ADR cell lines (the latter shows fourfold increased protein tyrosine kinase activity) except for the compds. formed from 6-quinolinecarboxaldehyde and malononitrile and 7-quinolinecarboxaldehyde and cyanoacetamide, which showed a significant (11- and 42-fold, resp.) increase in potency against the MCF7/ADR cell line. Furthermore, no association was found between growth inhibition and inhibition of the EGFR protein tyrosine kinase (PTK), using a cell-free assay. In addition, new compds. were prepared from 2- and 4-quinolinecarboxaldehyde with extended conjugation in the side chains or with methoxypolyethoxyethyl esters in the side chain to increase water solubility. These compds. showed substantial cytotoxicity, with IC50 values in the range 1-25  $\mu$ M, but similar values were observed against both cell lines. No association was found between inhibition of PTK and growth inhibition, again indicating that their mode of action may not be specific for the EGF receptor.

- CC 27-17 (Heterocyclic Compounds (One Hetero Atom))  
Section cross-reference(s): 1
- ST quinoline tyrphostin deriv prepn antiproliferative activity; cytotoxicity  
quinoline tyrphostin deriv; Knoevenagel condensation  
quinolinecarboxaldehyde malononitrile deriv
- IT Structure-activity relationship  
(antiproliferative; synthesis and antiproliferative activity of unsatd. quinoline derivs.)
- IT Antitumor agents  
Cytotoxicity  
(synthesis and antiproliferative activity of unsatd. quinoline derivs.)
- IT Epidermal growth factor receptors  
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)  
(synthesis and antiproliferative activity of unsatd. quinoline derivs.)
- IT 4363-93-3, 4-Quinolinecarboxaldehyde 172678-61-4  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(Knoevenagel condensation with malononitrile derivative)
- IT 4113-04-6, 6-Quinolinecarboxaldehyde 5470-96-2, 2-Quinolinecarboxaldehyde 24571-64-0 38707-70-9, 8-Quinolinecarboxaldehyde 49573-30-0, 7-Quinolinecarboxaldehyde  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(Knoevenagel condensation with malononitrile derivs.)
- IT 78429-16-0  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(Knoevenagel condensation with quinolinecarboxaldehyde derivative)
- IT 105-34-0, Methyl cyanoacetate 105-56-6, Ethyl cyanoacetate 107-91-5, 2-Cyanoacetamide 109-77-3, Malononitrile 868-54-2 5459-58-5, Butyl cyanoacetate 7357-70-2, 2-Cyanothioacetamide  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(Knoevenagel condensation with quinolinecarboxaldehydes)
- IT 372-09-8, 2-Cyanoacetic acid  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(condensation reaction with (methoxyethoxy)ethoxy ethanol)
- IT 112-35-6, 2-(2-(2-Methoxyethoxy)ethoxy)ethanol 9004-74-4, Methoxypolyethyleneglycol  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(condensation reaction with cyanoacetic acid)
- IT 182615-11-8P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and Knoevenagel condensation with quinolinecarboxaldehyde)
- IT 315178-31-5P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and Knoevenagel condensation with quinolinecarboxaldehydes)
- IT 127635-74-9P 315178-03-1P 315178-04-2P 315178-05-3P 315178-06-4P 315178-07-5P 315178-08-6P 315178-09-7P 315178-10-0P 315178-11-1P

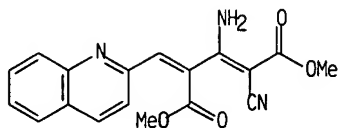
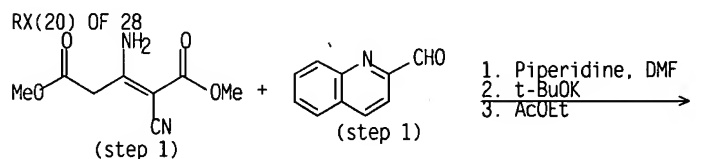
315178-12-2P 315178-13-3P 315178-14-4P 315178-15-5P 315178-16-6P  
 315178-17-7P 315178-18-8P 315178-19-9P 315178-20-2P 315178-21-3P  
 315178-22-4P 315178-23-5P 315178-24-6P 315178-25-7P 315178-26-8P  
 315178-27-9P 315178-28-0P 315178-29-1P 315178-30-4P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

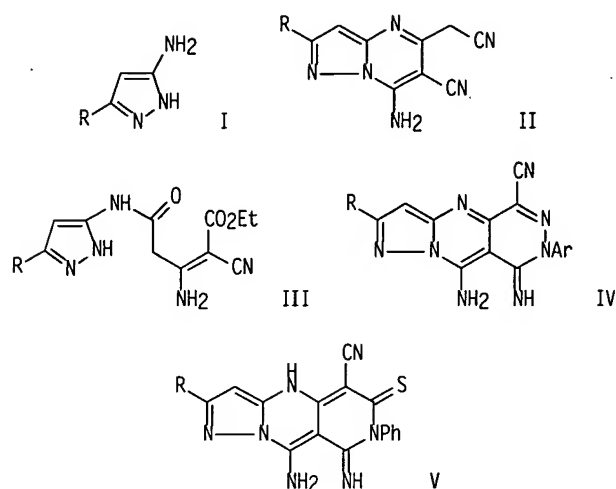
(synthesis and antiproliferative activity of unsatd. quinoline derivs.)

## RETABLE

Referenced Author (RAU)	Year (RPY)	VOL (RVL)	PG (RPG)	Referenced Work (RWK)	Referenced File
Akasaki, Y	1989			Japanese Patent Appl	
Brunton, V	1994	9	291	Anti-Cancer Drug Des	CAPLUS
Brunton, V	1996	11	265	Anti-Cancer Drug Des	CAPLUS
Brunton, V	1996	11	463	Anti-Cancer Drug Des	CAPLUS
Carmichael, J	1987	47	936	Cancer Research	CAPLUS
Carsky, P	1980	2	291	Liebigs Annalen der	
Casnellie, J	1982	72	282	Proceedings of the N	
Fatiadi, A	1978		165	Synthesis	CAPLUS
Gazit, A	1989	32	2344	Journal of Medicinal	CAPLUS
Gazit, A	1991	34	1897	Journal of Medicinal	
Gazit, A	1993	36	3556	Journal of Medicinal	CAPLUS
Junek, H	1976		999	Monatshefte fur Chem	
Kingsbury, W	1993	36	3308	Journal of Medicinal	CAPLUS
Klohs, W	1997	9	562	Current Opinions in	CAPLUS
Krause, M	1987	6	605	EMBO Journal	
McGown, A	1998	77	216	British Journal of C	CAPLUS
Mitzutani, T	1997	119	8991	Journal of the Ameri	
Rodionov, V	1944	14	330	Journal of General C	CAPLUS
Tulyganov, T	1982	18	604	Chemistry of Natural	
Workman, P	1992	3	369	Seminars in Cancer B	CAPLUS



L24 ANSWER 8 OF 28 CASREACT COPYRIGHT 2005 ACS on STN  
 AN 129:81707 CASREACT  
 TI Heterocyclic amidines: synthesis of new azaindene derivatives  
 AU Abdel-Aziz El-Taweel, Fathy Mohamed  
 CS Department of Chemistry, Faculty of Science, New Damietta, Egypt  
 SO Alexandria Journal of Pharmaceutical Sciences (1998), 12(1),  
 11-15  
 CODEN: AJPSSES; ISSN: 1110-1792  
 PB University of Alexandria, Faculty of Pharmacy  
 DT Journal  
 LA English  
 GI



AB 3-Substituted 5-aminopyrazole I (R = antipyrinyl, X = H) reacted differently with the enamines to give the pyrazolopyrimidine II and pyrazole derivative III. II reacted with arenediazonium chloride and Ph isothiocyanate to give pyrazolopyrimidinopyridazine IV and pyrazolopyrimidinopyridinethione V, resp. Other derivs. were also prepared

CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))

ST heterocyclic amidine prepn; azaindene prepn

IT Cyclization

(preparation of azaindene derivs.)

IT 96-33-3 100-34-5, Phenyl diazonium chloride 103-72-0, Phenyl isothiocyanate 105-56-6, Ethyl cyanoacetate 109-77-3, Malononitrile 539-74-2, Ethyl 3-bromopropanoate 868-54-2 879-72-1 2028-84-4, p-Tolyl diazonium chloride 2469-99-0, Acetylacetonitrile 28447-79-2 90475-84-6 99819-60-0 157040-90-9 209343-81-7

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of azaindene derivs.)

IT 99819-65-5P 209343-74-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of azaindene derivs.)

IT 209343-75-9P 209343-76-0P 209343-77-1P 209343-78-2P 209343-79-3P 209343-80-6P 209343-82-8P 209343-83-9P 209343-84-0P 209343-85-1P 209343-86-2P

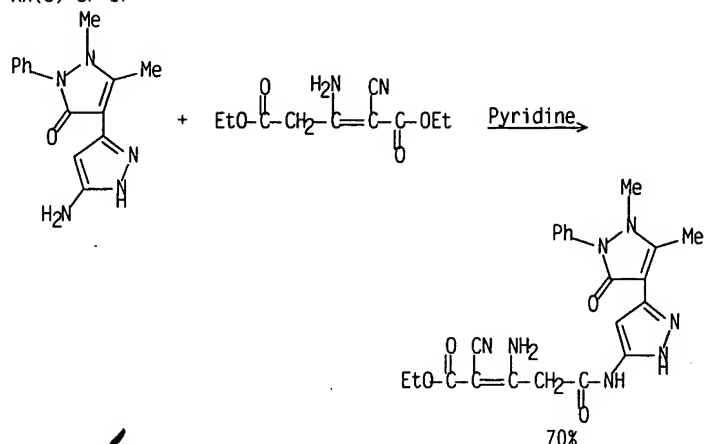
RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of azaindene derivs.)

RETABLE

Referenced Author (RAU)	Year (RPY)	VOL (RVL)	PG (RPG)	Referenced Work (RWK)	Referenced File
Behr, L	1967			Chemistry of Heteroc	
El-Taweel, F	1995	104	567	Bull Soc Chim Belg	CAPLUS
Elagamey, A	1984	317	289	Arch Pharm (Weinheim)	CAPLUS
Elmagdi, M	1987	41	320	Advances in Heterocy	
Elmagdi, M	1990	48	219	Advances in Heterocy	
Elmagdi, M	1990	63	1854	Bull Chem Soc (Jpn)	CAPLUS
Fahmy, S	1980	30	390	J Chem Techn Biotech	CAPLUS
Novinson, T	1974	17	645	J Med Chem	CAPLUS
Senga, K	1981	24	610	J Med Chem	CAPLUS
Sofan, M	1994	49	482	Pharmazie	CAPLUS

RX(3) OF 17



✓ L24 ANSWER 9 OF 28 CASREACT COPYRIGHT 2005 ACS on STN

AN 124:86826 CASREACT

TI Method of preparing 2,5-dimethyl-4-piperidone

IN Praliev, K. D.; Murzagulova, K. B.; Akhmedova, S. S.; Nurlibaev, A. K.;  
 Abdykalykova, R. A.; Sharifkanov, A. Sh.; Trubachev, V. I.; Yablokov, S.  
 K.; Turmukhanova, M. Zh.; Sagimbekova, N. B.

PA Anzhero-Sudzhenskii Khimfarmzavod, Russia

SO Russ.

From: Izobreteniya 1995, (1), 161-2.

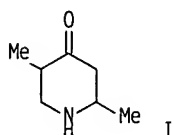
CODEN: RUXXE7

DT Patent

LA Russian

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	RU 2026289	C1	19950109	RU 1992-4941898	19920417
PRAI	SU 1992-4941898		19920417		
GI					



AB The title compound (I) is prepared from NH<sub>3</sub> and a starting oxo compound [CH<sub>3</sub>COCH<sub>2</sub>CO<sub>2</sub>Et; (II)] via cyclization at elevated temps. II is treated with NH<sub>3</sub>, and the resulting amine [CH<sub>3</sub>(H<sub>2</sub>N)C:CHCO<sub>2</sub>Et] is hydrogenated over a Ni catalyst at 60-80 atm and 35-40.degree.. The obtained CH<sub>3</sub>CH(NH<sub>2</sub>)CH<sub>2</sub>CO<sub>2</sub>Et reacts with CH<sub>2</sub>:CMeCO<sub>2</sub>Me at mol ratio 1:(2-5) in the presence of an acidic catalyst and a protic solvent at 90-100.degree., followed by cyclization in the presence of tech. NaOMe, with simultaneous heating and evaporation of formed MeOH and EtOH, to give I.

IC ICM C07D211-74

CC 27-16 (Heterocyclic Compounds (One Hetero Atom))

Section cross-reference(s): 45

ST dimethylpiperidone; piperidone dimethyl; acetoacetate reductive amination;  
 aminobutyrate cyclocondensation methacrylate

IT 5303-65-1P, .beta.-Aminobutyric acid ethyl ester 7318-00-5P.

.beta.-Aminocrotonic acid ethyl ester

RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (intermediate; preparation of dimethylpiperidone)

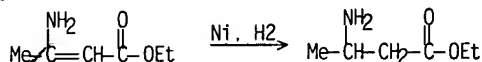
IT 4558-87-6P, 2,5-Dimethyl-4-piperidone

RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation) (preparation of dimethylpiperidone)

IT 80-62-6, Methyl methacrylate 141-97-9, Ethyl acetoacetate 7664-41-7, Ammonia, reactions

RL: RCT (Reactant); RACT (Reactant or reagent) (starting material; preparation of dimethylpiperidone)

RX(3) OF 6



NOTE: 35-40.degree. and 60-80 atm

✓ L24 ANSWER 10 OF 28 CASREACT COPYRIGHT 2005 ACS on STN

AN 123:111939 CASREACT

TI Reactions of polyfunctional amines with 3-amino-4-(anilinothiomethylidene)-2-cyano-2-pentenedioic acid diethyl ester

AU Winnik, Witold

CS Department of Chemistry, Cleveland State University, Cleveland, OH, 44115, USA

SO Journal of Heterocyclic Chemistry (1995), 32(2), 477-82

CODEN: JHTCAD; ISSN: 0022-152X

PB HeteroCorporation

DT Journal

LA English

AB 3-Amino-4-(anilinothiomethylene)-2-cyano-2-pentenedioic acid di-Et ester reacts with ethylenediamine, 1,3-propylenediamine and 1,4-butylenediamine bicyclic cyclocondensation products. The title compound reacts with diethylenetriamine and 2-(2-aminoethylamino)ethanol to give new seven membered ring tricyclic compds. The mechanism for these reactions is discussed.

CC 28-9 (Heterocyclic Compounds (More Than One Hetero Atom))

Section cross-reference(s): 22, 26, 27

ST condensation diamine aminopentenedioate; cyclocondensation diamine aminopentenedioate

IT Addition reaction

Cyclocondensation reaction

Elimination reaction

(cyclocondensation of diamines with (amino)cyano[(methylthio)(phenylamino)methylene]pentenedioate)

IT Amines, reactions

RL: RCT (Reactant); RACT (Reactant or reagent)

(di-, cyclocondensation of diamines with (amino)cyano[(methylthio)(phenylamino)methylene]pentenedioate)

IT 107-15-3, 1,2-Ethanediamine, reactions 109-76-2, 1,3-Propanediamine

110-60-1, 1,4-Butanediamine 111-40-0, Diethylenetriamine 111-41-1,

2-[(2-Aminoethyl)amino]ethanol 2651-09-4, 2-Amino-2-cyano-2-pentenedioic

acid dimethyl ester 7664-41-7, Ammonia, reactions 154227-73-3,

2-Pentenedioic acid, 3-amino-2-cyano-4-[(methylthio)(phenylamino)methylene]-, diethyl ester, (E,Z)

RL: RCT (Reactant); RACT (Reactant or reagent)

(cyclocondensation of diamines with (amino)cyano[(methylthio)(phenylamino)methylene]pentenedioate)

IT 165684-93-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

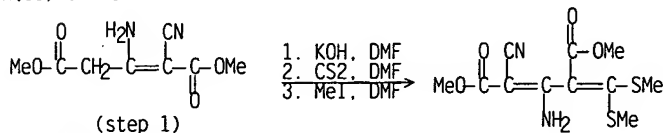
(cyclocondensation of diamines with (amino)cyano[(methylthio)(phenylamino)methylene]pentenedioate)

IT 165684-85-5P 165684-86-6P 165684-87-7P 165684-88-8P 165684-89-9P  
165684-90-2P 165684-91-3P 165684-92-4P

RL: SPN (Synthetic preparation); PREP (Preparation)

(cyclocondensation of diamines with (amino)cyano[(methylthio)(phenylamino)methylene]pentenedioate)

RX(11) OF 13



L24 ANSWER 11 OF 28 CASREACT COPYRIGHT 2005 ACS on STN

AN 120:244934 CASREACT

TI Investigation of isothiocyanate addition to alkylidene derivatives of malononitrile and cyanoacetic acid esters

AU Hehemann, David G.; Winnik, Witold

CS Dep. Chem., Cleveland State Univ., Cleveland, OH, 44115, USA

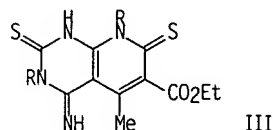
SO Journal of Heterocyclic Chemistry (1993), 30(4), 887-91

CODEN: JHTCAD; ISSN: 0022-152X

DT Journal

LA English

GI



AB Addition of aryl isothiocyanates RNCS (I; R = Ph, 4-ClC6H4) to activate methylene compds. leads to a variety of compds. depending on the structure of the starting material and conditions used to conduct the addition. Addition of I to R1C(CN):CMeCH2CO2Et (II; R1 = CN) leads to pyrido[2,3-d]pyrimidine III, resulting from addition of a second mole of cyanate to the initial adduct. Addition of I to II (R1 = CO2Et) led to a mixture of pyridine and thiopyran adducts, while addition of I to EtO2CC(CN):C(NH2)CH2CO2Et led to open chain structures.

CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))

Section cross-reference(s): 27

ST addn aryl isothiocyanate active methylene; cycloaddn aryl isothiocyanate alkylidenemalononitrile alkylidenecyanoacetate

IT Cycloaddition reaction

(of aryl isothiocyanates with alkylidenemalononitrile and alkylidenecyanoacetate derivs. to pyridopyrimidines, pyridine, and thiopyran derivs.)

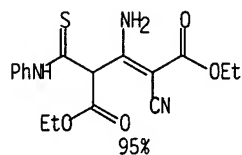
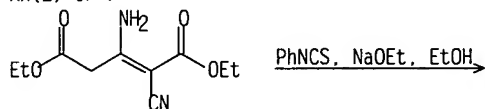
IT 103-72-0, Phenyl isothiocyanate

RL: RCT (Reactant); RACT (Reactant or reagent)

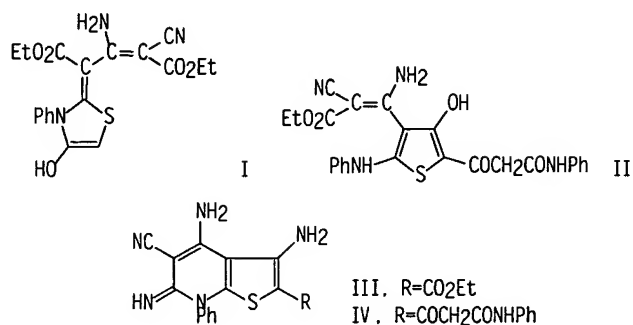
(addition and cycloaddn. with alkylidenemalononitrile and

- alkylidenecyanoacetate derivs.)
- IT 145909-72-4  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(addition with aryl isothiocyanates)
- IT 2131-55-7, 4-Chlorophenyl isothiocyanate  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(cycloaddn. with alkylidenemalononitrile and alkylidenecyanoacetate derivs.)
- IT 52903-67-0 89516-23-4 89516-30-3  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(cycloaddn. with aryl isothiocyanates)
- IT 154227-63-1P 154227-64-2P 154227-65-3P 154227-66-4P 154227-68-6P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and S-methylation of)
- IT 154227-71-1P 154227-72-2P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and desulfurization of)
- IT 154227-69-7P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation and rearrangement to pyridone derivative)
- IT 154227-70-0P 154227-73-3P 154227-74-4P 154227-75-5P 154227-76-6P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RX(2) OF 7



✓ L24 ANSWER 12 OF 28 CASREACT COPYRIGHT 2005 ACS on STN  
AN 117:69755 CASREACT  
TI Phenyl isothiocyanate in heterocyclic synthesis: novel synthesis of thiazoles, thieno[2.3-b]pyridine, thiophene and thieno[3.2-c]pyridazine derivatives  
AU Mohareb, Rafat Milad  
CS Fac. Sci., Cairo Univ., Giza, Egypt  
SO Monatshefte fuer Chemie (1992), 123(4), 341-7  
CODEN: MOCMB7; ISSN: 0026-9247  
DT Journal  
LA English  
GI



AB The enamino nitriles EtO<sub>2</sub>CCH<sub>2</sub>C(NH<sub>2</sub>):C(CN)CO<sub>2</sub>Et and (NC)<sub>2</sub>C:C(NH<sub>2</sub>)CH<sub>2</sub>CN react with PhNCS followed by cyclization with .alpha.-halo ketones ClCH<sub>2</sub>CO<sub>2</sub>Et and BrCH<sub>2</sub>COCH<sub>2</sub>CONHPh to afford in each case thiazole I, thiophene II and the thieno[2,3-b]pyridine derivs. III and IV. Chemical and spectroscopic evidence for the structures of the new compds. is described.

CC 28-2 (Heterocyclic Compounds (More Than One Hetero Atom))

ST cyclization isothiocyanate enamino nitrile halo ketone; thiazole; thienopyridine; thiophene; thienopyridazine

IT Ring closure and formation

(of enamino nitriles with Ph isothiocyanate and haloketones)

IT 82754-70-9 82754-71-0

RL: RCT (Reactant); RACT (Reactant or reagent)  
(cyclization of, with Ph isothiocyanate)

IT 868-54-2 1118-60-1 28447-79-2

RL: RCT (Reactant); RACT (Reactant or reagent)  
(cyclization of, with Ph isothiocyanate and haloketones)

IT 105-39-5, Ethyl chloroacetate 1205-74-9

RL: RCT (Reactant); RACT (Reactant or reagent)  
(cyclization of, with enamino nitriles and Ph isothiocyanate)

IT 103-72-0, Phenyl isothiocyanate

RL: RCT (Reactant); RACT (Reactant or reagent)  
(cyclization of, with enamino nitriles and haloketones)

IT 142168-48-7P 142168-49-8P 142168-51-2P 142168-52-3P 142168-53-4P

142168-56-7P 142168-58-9P 142168-59-0P 142168-60-3P  
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
(preparation and spectra of)

IT 142168-54-5P 142168-55-6P

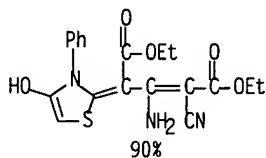
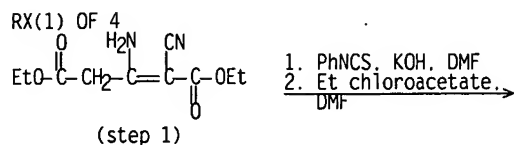
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

IT 142168-57-8P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation, spectra and cyclization of)

IT 142168-47-6P 142168-50-1P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation, spectra and reactions of)



L24 ANSWER 13 OF 28 CASREACT COPYRIGHT 2005 ACS on STN

AN 113:97104 CASREACT

TI The structure of products of coupling of arenediazonium salts with 3-aminocrotononitrile derivatives

AU Elnagdi, Mohamed Hilmy; Sadek, Kamal Usef; Taha, Nadia Mohamed; Yassin, Youssef Mahfous

CS Chem. Dep., Cairo Univ., Giza, Egypt

SO Collection of Czechoslovak Chemical Communications (1990),

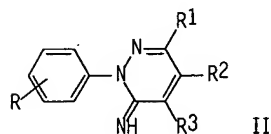
55(3), 734-44

CODEN: CCCCAK; ISSN: 0010-0765

DT Journal

LA English

GI



AB The coupling reaction of RC<sub>6</sub>H<sub>4</sub>N<sub>2</sub>+C1- (R = H, 4-Me, 4-MeO, 2-Cl, 4-Cl) with RICH<sub>2</sub>CR<sub>2</sub>:CR<sub>3</sub>CN (R<sub>1</sub>, R<sub>3</sub> = CN, CO<sub>2</sub>Et; R<sub>2</sub> = NH<sub>2</sub>, Ph) gave RC<sub>6</sub>H<sub>4</sub>NHN:CR<sub>1</sub>CR<sub>2</sub>:CR<sub>3</sub>CN (I). Spectral data and chemical behavior indicate that the hydrazone I is in the (E)-form. The cyclization of I to give pyridazines, e.g., II, is also reported.

CC 25-5 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds) Section cross-reference(s): 28

ST aryldiazonium coupling aminocrotonitrile; cyanohydrazone cyclization; pyridazine imino aryl

IT Coupling reaction  
(of aryldiazonium chlorides with aminocrotononitrile derivs., hydrazones from)

IT Ring closure and formation  
(of cyanohydrazones, pyridazines from)

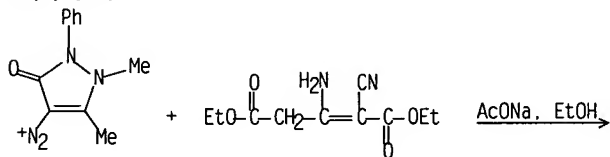
IT Diazonium compounds  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(arene, salts, coupling of, with aminocrotononitrile derivs., hydrazones from)

IT Hydrazones  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(cyano, cyclization of, pyridazines from)

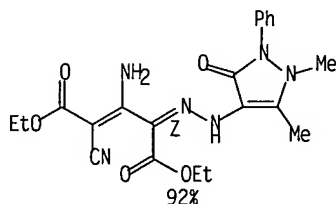
IT 89-90-7 100-34-5 2028-74-2 2028-84-4 4346-59-2 95610-53-0  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(coupling of, with aminocrotononitrile derivs., hydrazones from)

IT 868-54-2 28447-79-2 86165-77-7 101685-29-4  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (coupling of, with aryldiazonium chlorides, hydrazones from)  
 IT 128755-87-3P 128755-88-4P 128755-89-5P 128755-90-8P 128755-93-1P  
 128755-95-3P 128755-96-4P 128755-97-5P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (preparation and cyclization of, pyridazine from)  
 IT 128755-83-9P 128755-84-0P 128755-85-1P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (preparation and cyclization of, pyridazines and pyridines from)  
 IT 74982-79-9P 82315-80-8P 82754-65-2P 101685-31-8P 109613-82-3P  
 124612-51-7P 124612-52-8P 128755-86-2P 128755-91-9P 128755-92-0P  
 128755-94-2P 128755-98-6P 128755-99-7P 128756-00-3P 128756-01-4P  
 128756-02-5P 128756-03-6P 128756-04-7P 128756-05-8P 128756-06-9P  
 128756-07-0P 128756-08-1P 128784-62-3P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)

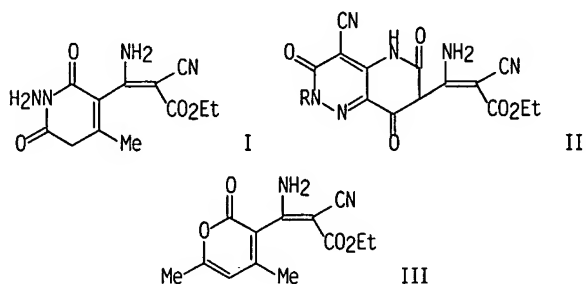
RX(2) OF 9



Cl-

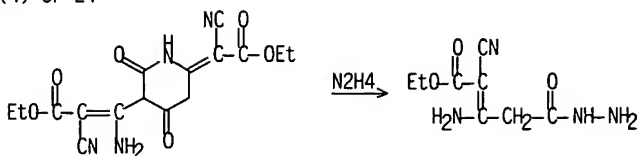


L24 ANSWER 14 OF 28 CASREACT COPYRIGHT 2005 ACS on STN  
 AN 111:39155 CASREACT  
 TI A convenient synthesis of ethyl .beta.-dioxohydropyridinyl-, ethyl  
 .beta.-dihydrodioxopyrido[3.2-c]pyridazinyl- and ethyl  
 .beta.-oxopyranylacrylate derivatives  
 AU Abdel Galil, Fathy M.; Hashim, Obeyes K.; Saleh, Sohair S.  
 CS Fac. Sci., Cairo Univ., Giza, Egypt  
 SO Heterocycles (1988), 27(10), 2301-4  
 CODEN: HETCYAM; ISSN: 0385-5414  
 DT Journal  
 LA English  
 GI

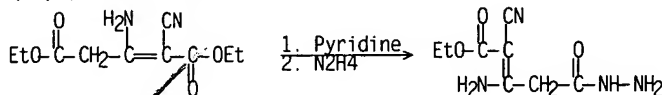


- AB Various pyridines, e.g., I, pyrido[3.2-c]pyridazines, e.g., II (R = Ph, 4-MeC<sub>6</sub>H<sub>4</sub>, 4-BrC<sub>6</sub>H<sub>4</sub>), and pyrans, e.g. III, were prepared from di-Et 3-amino-2-cyano-2-pentenedioate.
- CC 27-16 (Heterocyclic Compounds (One Hetero Atom))
- ST aminocyanopyridylacrylate deriv; pyridopyridazinetrione  
aminocyanooethoxycarbonylviny; pyranone aminocyanooethoxycarbonylviny;  
pyridinedione aminocyanooethoxycarbonylviny; aminocyanopentenedioate  
cyclocondensation acetoacetate pentanedione; dimerization  
aminocyanopentenedioate
- IT Cyclocondensation reaction  
(of aminocyanopentenedioate hydrazide with diketo compds..  
heterocyclics from)
- IT 100-34-5, Benzene diazonium chloride 2028-84-4, p-Toluene diazonium  
chloride 2028-85-5, p-Bromobenzene diazonium chloride  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(coupling of, with pyridinedione derivative)
- IT 123-54-6, Acetylacetone, reactions 141-97-9, Ethyl acetoacetate  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(cyclocondensation of, with aminocyanopentenedioate hydrazide)
- IT 82754-71-0  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(cyclocondensation of, with pentanedione or acetylacetate)
- IT 121359-23-7P 121359-26-0P 121359-27-1P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)  
(preparation and cyclization of, pyridopyridazinetrione from)
- IT 121359-22-6P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)  
(preparation and reactions of, with arenediazonium chlorides)
- IT 121359-24-8P 121359-25-9P 121359-28-2P 121377-18-2P 121377-19-3P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)
- IT 28447-79-2, Diethyl 3-amino-2-cyano-2-pentenedioate  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(self cyclocondensation of)

RX(4) OF 24



RX(12) OF 24 - 2 STEPS



L24 ANSWER 15 OF 28 CASREACT COPYRIGHT 2005 ACS on STN

AN 110:135171 CASREACT

TI Syntheses with nitriles. LXXIX. Methyl 3-amino-4-carbamoyl-2-cyano-2-butenate, a dimer of methyl cyanoacetate and cyanoacetamide

AU Junek, Hans; Sarhan, El Taher; Sterk, Heinz

CS Inst. Org. Chem., Karl Franzens Univ., Graz, A-8010, Austria

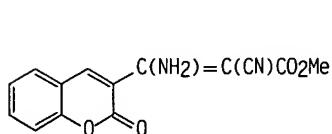
SO Monatshefte fuer Chemie (1988), 119(6-7), 717-26

CODEN: MOCMB7; ISSN: 0026-9247

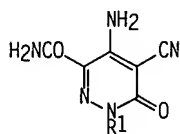
DT Journal

LA German

GI



II



III

AB RNHCOCH2C(NH2):CH(CN)CO2Me (I, R = H) was prepared by amidation of the diester. The dimethylamide and I (R = Ph, substituted Ph) were similarly prepared. Reaction of I (R = H) with 2-HOC6H4CHO gave pyrone II. I (R = H) reacted with R1N2+Cl- (R1 = Ph, substituted Ph) to give pyridazinones III.

CC 28-15 (Heterocyclic Compounds (More Than One Hetero Atom))

ST carbamoylcyanoacetate prepn reaction; pyridinone; pyridazinone

IT 87-62-7, 2,6-Dimethylaniline 88-17-5, 2-Trifluoromethylaniline

95-68-1, 2,4-Dimethylaniline 98-16-8, 3-Trifluoromethylaniline

104-94-9, 4-Methoxyaniline 108-42-9, 3-Chloroaniline 108-44-1,

3-Methylaniline, reactions 121-50-6, 2-Chloro-5-trifluoromethylaniline

536-90-3, 3-Methoxyaniline

RL: RCT (Reactant); RACT (Reactant or reagent)

(amidation by, of aminocyanoglutaconate)

IT 78429-16-0

RL: RCT (Reactant); RACT (Reactant or reagent)

(amidation of)

IT 119689-97-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and hydrolysis of)

IT 110568-62-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reactions of)

IT 119689-94-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)

(preparation and ring closure of)

IT 531-81-7P 15828-10-1P 87831-20-7P 99657-96-2P 119689-86-0P  
 119689-87-1P 119689-88-2P 119689-89-3P 119689-90-6P 119689-91-7P  
 119689-92-8P 119689-93-9P 119689-95-1P 119689-96-2P 119689-98-4P  
 119689-99-5P 119690-00-5P 119690-01-6P 119690-02-7P

RL: SPN (Synthetic preparation); PREP (Preparation)

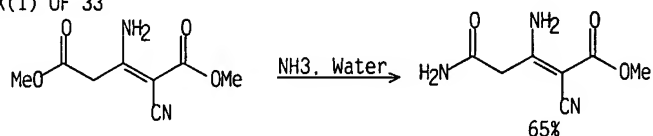
(preparation of)

IT 90-02-8, Salicylaldehyde, reactions 100-34-5, Benzenediazonium chloride  
 2028-72-0, 3-Methylbenzenediazonium chloride 4346-59-2,  
 4-Methoxybenzenediazonium chloride 53559-94-7, 2,4-Dimethylbenzene  
 diazonium chloride

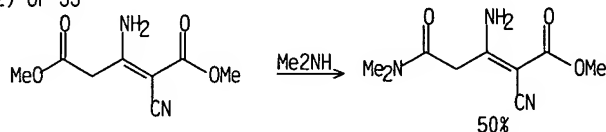
RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction of, with aminocyanoglutaconamide)

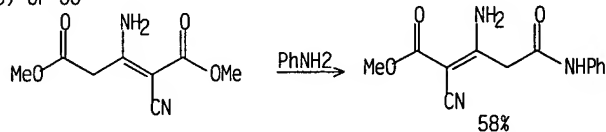
RX(1) OF 33



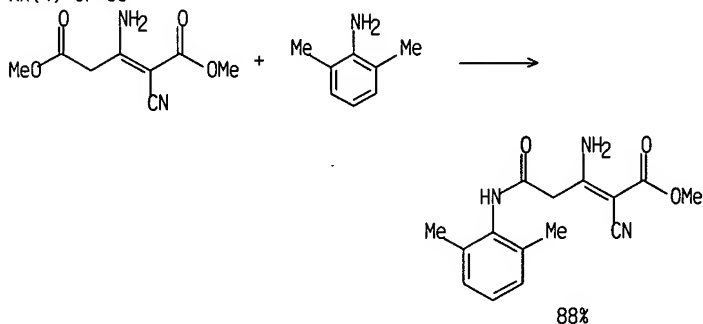
RX(2) OF 33

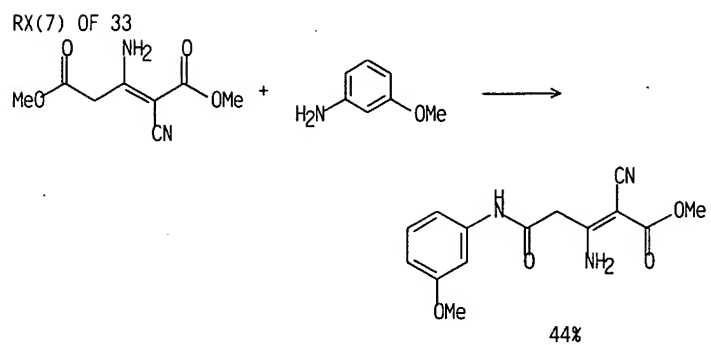
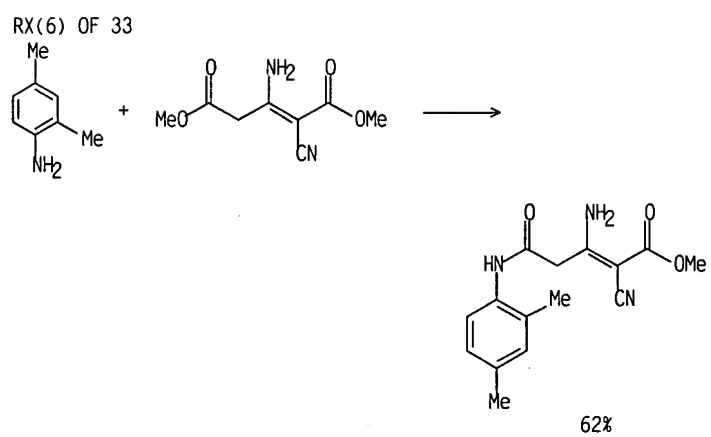
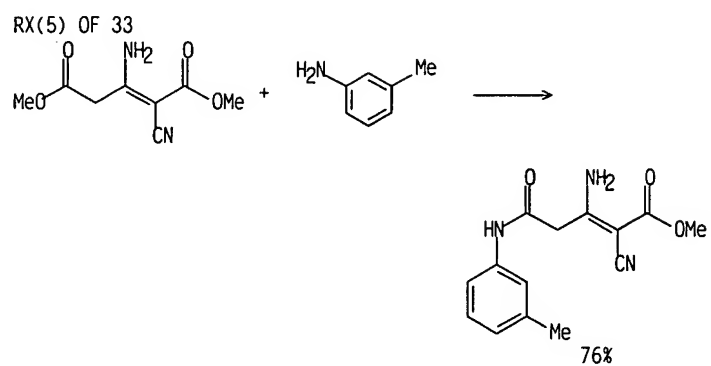


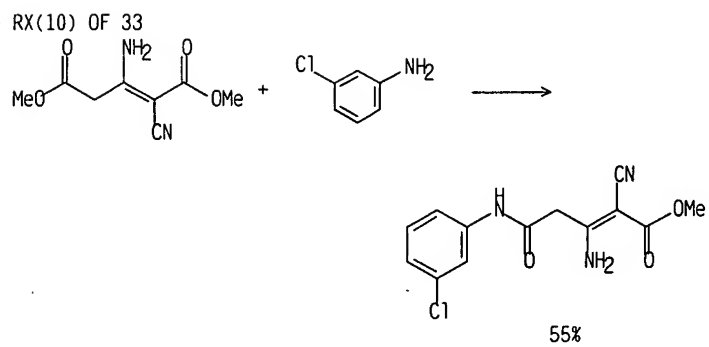
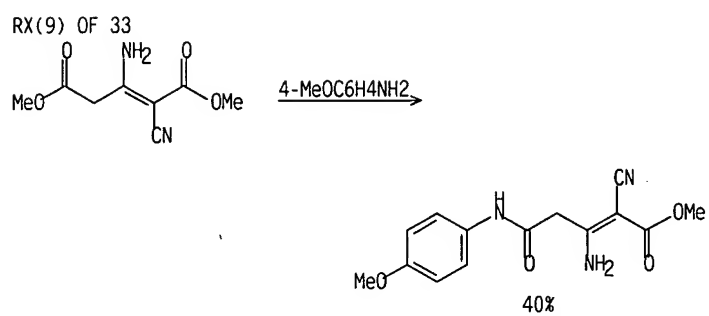
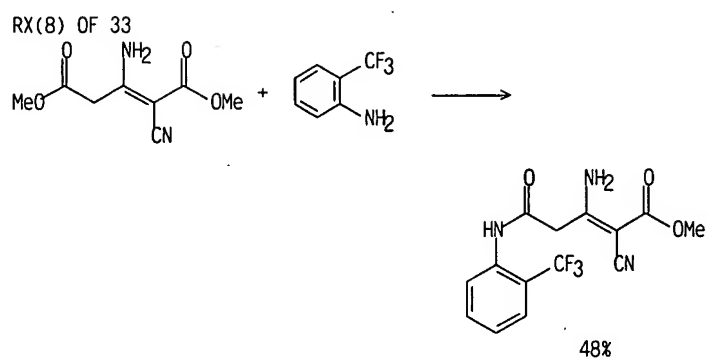
RX(3) OF 33

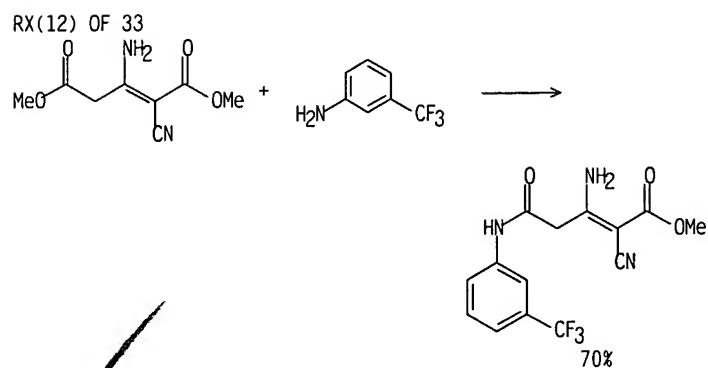
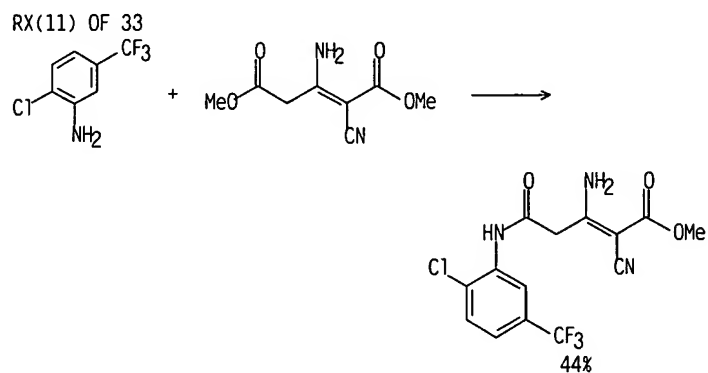


RX(4) OF 33

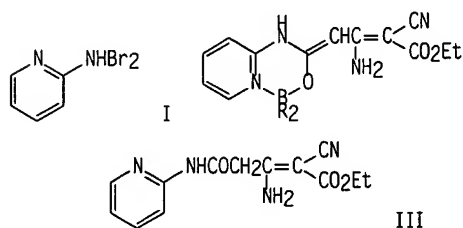








✓  
 E24 ANSWER 16 OF 28 CASREACT COPYRIGHT 2005 ACS on STN  
 AN 109:93090 CASREACT  
 TI Condensation of ethyl cyanoacetate with dialkylboryl derivatives of 2-aminopyridine  
 AU Dorokhov, V. A.; Baranin, S. V.  
 CS Inst. Org. Khim. im. Zelinskogo, Moscow, USSR  
 SO Izvestiya Akademii Nauk SSSR, Seriya Khimicheskaya (1987), (4), 954-5  
 CODEN: IASKA6; ISSN: 0002-3353  
 DT Journal  
 LA Russian  
 GI



AB Condensing NCCH<sub>2</sub>CO<sub>2</sub>Et with borylaminopyridines I (R = Pr, Bu) gave

chelates II, which on refluxing in EtOH gave pyridine III. Treating III with R<sub>2</sub>BSBu gave II.

CC 29-4 (Organometallic and Organometalloidal Compounds)

Section cross-reference(s): 27

ST condensation cyanoacetate borylaminopyridine; chelate borylpyridine; pentenoate pyrrolidylamino cyano

IT Condensation reaction

(of Et cyanoacetate with borylaminopyridines)

IT 105-56-6, Ethyl cyanoacetate

RL: RCT (Reactant); RACT (Reactant or reagent)

(condensation reaction of, with (borylamino)pyridines)

IT 37907-41-8 37907-43-0

RL: RCT (Reactant); RACT (Reactant or reagent)

(condensation reaction of, with Et cyanoacetate)

IT 115713-53-6P 115713-54-7P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation and deborylation of)

IT 115103-37-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reaction of, with butyltolylboranes)

IT 115103-38-3P 115103-39-4P

RL: SPN (Synthetic preparation); PREP (Preparation)

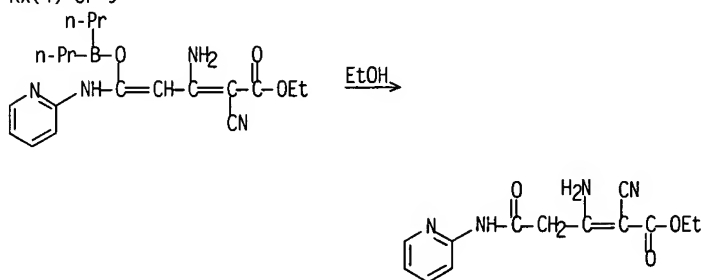
(preparation of)

IT 2938-91-2 2938-93-4

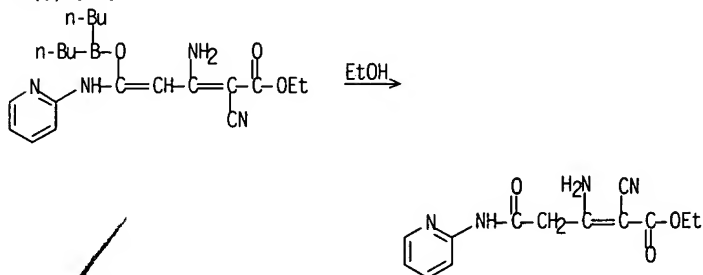
RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction of, with aminocyanooxo(pyridylamino)pentenoate)

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RX(5) OF 9

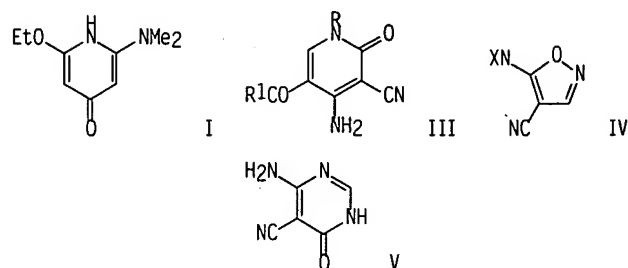


L24 ANSWER 17 OF 28 CASREACT COPYRIGHT 2005 ACS on STN

AN 107:96670 CASREACT

TI Functionalized enamines in the synthesis of some heterocyclic compounds

AU Golic, Ljubo; Stropnik, Crtomir; Stanovnik, Branko; Tisler, Miha  
 CS Dep. Chem., E. Kardelj Univ., Ljubljana, 61000, Yugoslavia  
 SO Heterocycles (1987), 25(1), 347-58  
 CODEN: HTCYAM; ISSN: 0385-5414  
 DT Journal  
 LA English  
 GI



AB Condensation of  $\text{EtOC}(\text{NH}_2):\text{CHCO}_2\text{Et}$  with  $\text{MeC}(\text{OMe})_2\text{NMe}_2$  gave 78% pyridinone I. Mol. structure of I was determined by x-ray crystallog. Condensation of  $\text{EtO}_2\text{CCH}_2\text{C}(\text{NH}_2):\text{C}(\text{CN})\text{CO}_2\text{Et}$  with  $\text{HC}(\text{OEt})_3$  gave  $\text{EtO}_2\text{CC}(\text{CHOEt})\text{C}(\text{NH}_2):\text{C}(\text{CN})\text{CO}_2\text{Et}$  (II). With  $\text{N}_2\text{H}_4$ , ethanolic  $\text{NH}_3$  and  $\text{EtNH}_2$ , II gave pyridinones III ( $\text{R} = \text{NH}_2$ ;  $\text{R}_1 = \text{OEt}$ ;  $\text{R} = \text{H}$ ,  $\text{R}_1 = \text{OEt}$ ;  $\text{R} = \text{Et}$ ,  $\text{R}_1 = \text{NHEt}$ ) resp. Similarly, condensation of aminoisoxazole IV ( $\text{X} = \text{H}_2$ ) with  $\text{Me}_2\text{NCH}(\text{OMe})_2$  gave IV ( $\text{X} = \text{CHNMe}_2$ ), which reacted with hot aqueous  $\text{NH}_3$  to give pyrimidinones V.

CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))  
 Section cross-reference(s): 75

ST aminoacrylate amide acetal cyclocondensation; aminopyridinone prepn  
 crystal structure; aminoisoxazole conversion pyridinone

IT Cyclocondensation reaction  
 (of aminosacrylate with amide acetals, pyridinones from)

IT Crystal structure  
 Molecular structure  
 (of dimethylaminopyridinone)

IT 504-29-0, 2-Aminopyridine  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (condensation of, with amide acetal)

IT 89779-30-6  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (condensation of, with amide acetal amidine from)

IT 34859-64-8 98027-17-9, 5-Amino-4-cyanoisoxazole  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (condensation of, with amide acetal, amidine from)

IT 109831-72-3  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (condensation of, with amide acetal, pyridinone from)

IT 67710-34-3  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (condensation of, with amide-acetal, amidine from)

IT 4637-24-5, N,N-Dimethylformamide dimethyl acetal 18871-66-4  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (condensation of, with aminoacrylates and aminoisoxazoles)

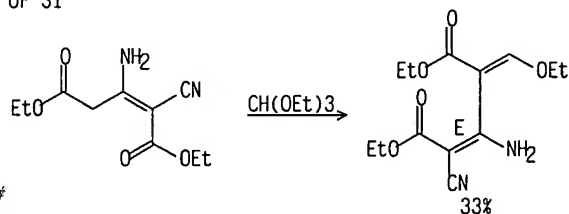
IT 109831-73-4P  
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
 (preparation and crystal structure of)

IT 109855-40-5P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (preparation and reaction of, with ammonia, pyridine from)

IT 109831-82-5P

- RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and reaction of, with ammonia, pyrimidinone from)
- IT 109831-74-5P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and reaction of, with ethylimine)
- IT 109831-84-7P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and reaction of, with hydrosene, amide from)
- IT 109831-76-7P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and reactions of, pyridinones from)
- IT 36171-99-0P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and reactions of, pyridyltriazole, bis(amidine) and thioacetamide from)
- IT 274-85-1P 6825-65-6P 38912-40-2P 57338-28-0P 109831-71-2P  
109831-75-6P 109831-77-8P 109831-79-0P 109831-80-3P 109831-81-4P  
109831-83-6P 109831-85-8P 109831-86-9P 109855-38-1P 109855-39-2P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)
- IT 109831-78-9  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with hydrogen-sulfide, diformylaminocrotonate from)
- IT 1640-73-9  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with hydroxylamine, triazolopyridine from)

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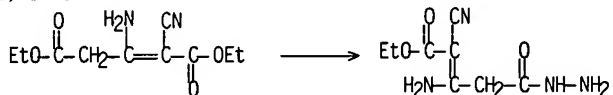
NOTE: 145.DEGREE.

- L24 ANSWER 18 OF 28 CASREACT COPYRIGHT 2005 ACS on STN  
AN 106:121381 CASREACT  
TI Dimerized ethyl cyanoacetate in heterocyclic dye synthesis: new pyridine azo dyes and tetrazole dyes  
AU Fahmy, Sherif M.; Mohareb, Rafat M.; Abd-All, Fatma A.  
CS Fac. Sci., Cairo Univ., Giza, Egypt  
SO Journal of Chemical Technology and Biotechnology (1986), 36(9), 410-14  
CODEN: JCTBED; ISSN: 0268-2575  
DT Journal  
LA English  
AB A variety of polyfunctional pyridine azo dyes and tetrazole dyes were prepared starting from Et cyanoacetate dimer [28447-79-2]. These derivs. dyed cellulose acetate, nylon 6, nylon 66, silk and wool with colors ranging from canary yellow to light violet.  
CC 41-3 (Dyes, Organic Pigments, Fluorescent Brighteners, and Photographic

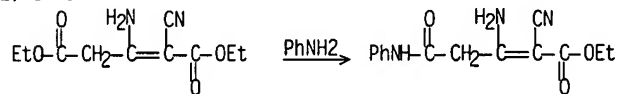
## Sensitizers)

- ST azo pyridine dye polyamide; tetrazole dye silk wool;  
aminocyanopentenedioate heterocyclic dye; acetate fiber azo dye
- IT Polyamide fibers, uses and miscellaneous  
RL: USES (Uses)  
(dyes for, pyridine azo and tetrazole derivs. as)
- IT Acetate fibers, uses and miscellaneous  
RL: USES (Uses)  
(dyes for, pyridine azo derivs. as)
- IT Dyeing  
(of acetate, polyamide, silk and wool with pyridine azo and tetrazole dyes)
- IT Dyes, azo  
(pyridine-containing, for acetate and polyamide fibers)
- IT Dyes  
(tetrazole derivs., for polyamide fibers)
- IT 9004-35-7  
RL: USES (Uses)  
(acetate fibers, dyes for, pyridine azo derivs. as)
- IT 62-53-3, Aniline, reactions  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(coupling of diazotized, with pyridine bases and dimerized Et cyanoacetate derivs.)
- IT 99636-48-3 105866-42-0 107140-23-8  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(cyclocondensation of)
- IT 15828-10-1P 82754-71-0P 99657-96-2P 105866-43-1P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and coupling of, with diazotized aniline)
- IT 87295-07-6P 99636-58-5P 104066-37-7P 105866-44-2P 105866-45-3P 105881-79-6P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of, as dye for polyamide fibers)
- IT 28447-79-2  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with nitrogen bases)

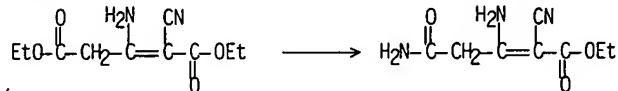
## RX(1) OF 8



## RX(2) OF 8

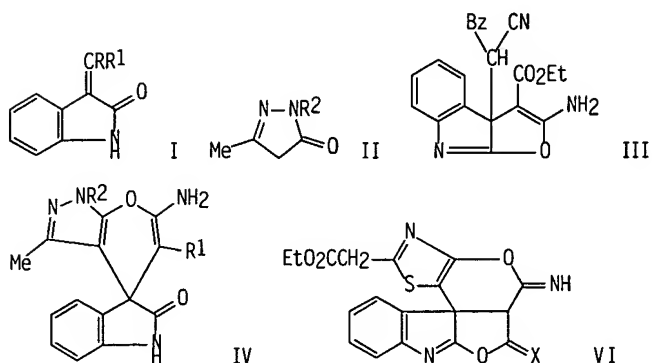


## RX(4) OF 8



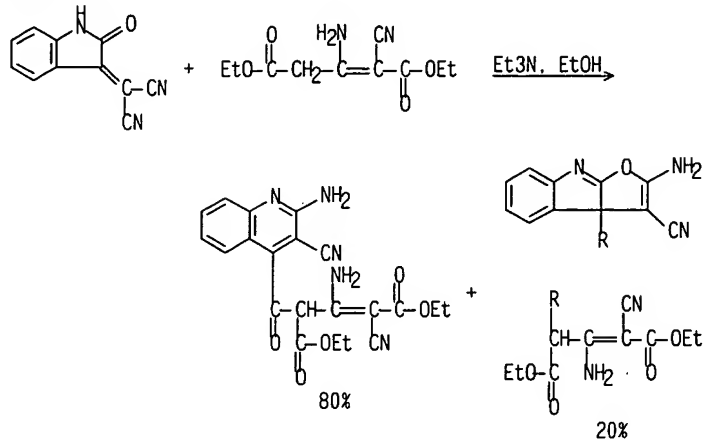
L24 ANSWER 19 OF 28 CASREACT COPYRIGHT 2005 ACS on STN  
AN 106:67180 CASREACT  
TI Novel synthesis of furo[2,3-b]indole derivatives  
AU Abd El-Latif, Fathy Faheem; Gohar, Abd El Kareem Mohammed Nasr; Fahmy.

Atiat Mohammed: Badr, Mahmoud Zarif Amin  
 CS Fac. Sci., El-Minia Univ., Egypt  
 SO Bulletin of the Chemical Society of Japan (1986), 59(4), 1235-8  
 CODEN: BCSJAB; ISSN: 0009-2673  
 DT Journal  
 LA English  
 GI



- AB Reaction of indolinones I (R = cyano; R1 = R, CO2Et) with nucleophiles.  
 e.g. PhCOCH2CN or pyrazolinones II (R2 = H, Ph) gave furoindole III and  
 spiro compds. IV, resp. Reaction of I with Et thiazolinonylacetate V in  
 presence of Et3N gave thiazolopyranofuroindoles VI (X = NH, O).
- CC 28-8 (Heterocyclic Compounds (More Than One Hetero Atom))
- ST cyanomethyleneindolinone cycloaddn thiazolinone pyrazolinone; furoindole;  
 thiazolopyranofuroindole; spiroindolinepyranopyrazole
- IT Cycloaddition reaction  
 (of cyanomethyleneindolinones with active methylene compds.,  
 furoindoles by)
- IT Spiro compounds  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of spiroindolinepyranopyrazoles)
- IT 91-56-5, Isatin  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (cyclocondensation of, with aminocyanopentenedioate)
- IT 74647-55-5P 106536-34-9P 106536-35-0P 106536-36-1P 106536-37-2P  
 106536-38-3P 106536-39-4P 106536-40-7P 106536-41-8P 106549-16-0P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)
- IT 614-16-4  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, with isatin derivative)
- IT 89-25-8 108-26-9 877-87-2 28447-79-2  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, with isatin derivs.)
- IT 6623-89-8 59225-18-2  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, with thiazolinone and pyrazolinone)

RX(2) OF 9



L24 ANSWER 20 OF 28 CASREACT COPYRIGHT 2005 ACS on STN

AN 106:4964 CASREACT

TI Activated nitriles in heterocyclic synthesis. A novel synthesis of pyridine and pyridazine derivatives

AU Fahmy, Sherif Mahmoud; Mohareb, Rafat Milad

CS Fac. Sci., Cairo Univ., Giza, Egypt

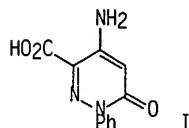
SO Synthesis (1985), (12), 1135-7

CODEN: SYNTBF; ISSN: 0039-7881

DT Journal

LA English

GI



AB The dimerization of NCCH<sub>2</sub>CONH<sub>2</sub> gave HO<sub>2</sub>CC(NH<sub>2</sub>):C(CN)CONH<sub>2</sub> which cyclized with CH<sub>2</sub>(COMe)<sub>2</sub>PhCH:CRCN (R = cyano, CO<sub>2</sub>Et), and EtOCH:C(CN)CO<sub>2</sub>Et to give pyridine derivs. and with PhN<sub>2</sub>+Cl<sup>-</sup> to give the pyridazine I.

CC 28-15 (Heterocyclic Compounds (More Than One Hetero Atom))

Section cross-reference(s): 27

ST pyridazinone aminocarboxy; pyridineylidenecyanoacetamide; cyanoacetamide dimerization; pentenedioic acid aminocyano

IT 107-91-5, Cyanoacetamide

RL: RCT (Reactant); RACT (Reactant or reagent) (dimerization of)

IT 105626-25-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation and hydrolysis of)

IT 105626-24-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation and reactions of)

IT 105626-26-4P 105626-27-5P 105626-28-6P 105626-29-7P 105626-30-0P

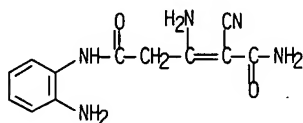
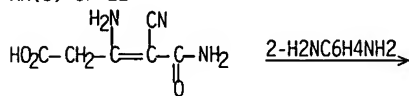
105626-31-1P 105626-32-2P 105626-33-3P 105626-34-4P 105626-35-5P

105626-36-6P 105626-37-7P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

IT 90-02-8, 2-Hydroxybenzaldehyde, reactions 94-05-3 95-54-5,  
o-Phenylenediamine, reactions 123-54-6, Acetyl acetone, reactions  
2025-40-3, Ethyl benzylidenecyanoacetate 2700-22-3, Benzalmalononitrile  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with aminocyanopentenedioamide)

RX(8) OF 22



✓ L24 ANSWER 21 OF 28 CASREACT COPYRIGHT 2005 ACS on STN

AN 104:206695 CASREACT

TI Syntheses with nitriles. LXXIV. 3-Amino-4,4-dicyano-3-butenoate, a synthetically useful dimer from malononitrile and cyanoacetate

AU Mittelbach, Martin; Junek, Hans

CS Inst. Org. Chem., Univ. Graz, Graz, A-8010, Austria

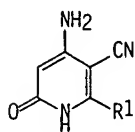
SO Liebigs Annalen der Chemie (1986), (3), 533-44

CODEN: LACHDL; ISSN: 0170-2041

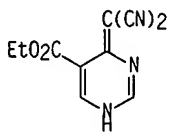
DT Journal

LA German

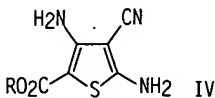
GI



II



III



AB Title dimer  $(\text{NC})_2\text{C}:\text{C}(\text{NH}_2)\text{CH}_2\text{CO}_2\text{R}$  (I, R = Me, Et) was prepared and its reactions were studied. Thus, I reacted with acids or bases to give 2(1H)-pyridones II ( $\text{R}_1 = \text{Cl}, \text{Br}, \text{OMe}, \text{OEt}$ ). Treatment of I with formamidine or sulfur gave pyrimidine and thiophene derivs. III and IV, resp. condensation reactions of I with benzaldehydes and with cyclopentanone were also studied. The  $\text{pK}_a$  value (10.15 at 25.degree.) of I (R = Et) was compared to that of related dimers.

CC 23-17 (Aliphatic Compounds)

Section cross-reference(s): 25, 27, 28

ST aminodicyanobutenoate prepn reaction; acidity aminodicyanobutenoate cyano; thiophene aminocyano; cyanobutenoate amino; butenoate aminodicyano; dimer malononitrile cyanoacetate; benzaldehyde condensation aminodicyanobutenoate; pyridone aminocyano; pyrimidine aminocyano

IT Acidity

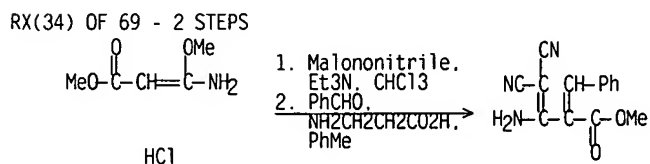
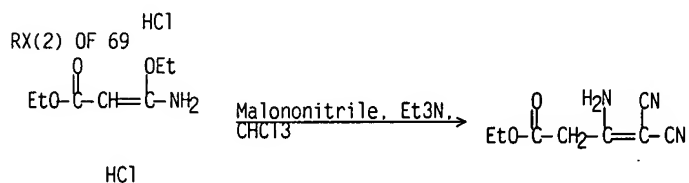
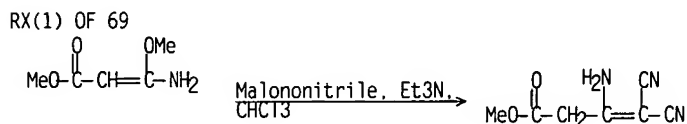
(constant, of aminodicyanobutenoate)

IT Dimers

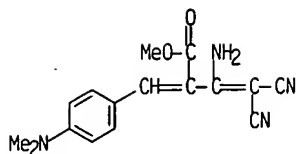
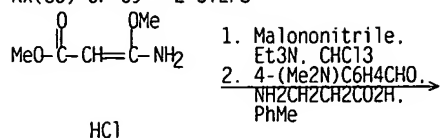
RL: SPN (Synthetic preparation); PREP (Preparation)

(of cyanoacetate and malononitrile, preparation and properties of)

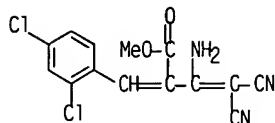
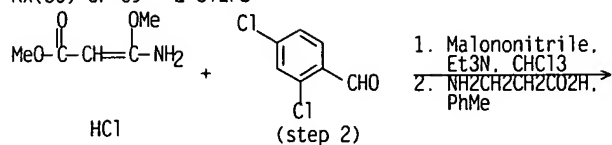
- IT 86-81-7 90-02-8, reactions 100-10-7 100-52-7, reactions 104-88-1, reactions 120-22-9 120-92-3 123-11-5, reactions 138-89-6 529-23-7 708-06-5 874-42-0 1122-91-4 1666-01-9 6313-33-3 10595-51-4  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (condensation of, with aminodicyanobutenoate)
- IT 109-77-3  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (condensation of, with aminoethoxyacrylate)
- IT 555-16-8, reactions 4637-24-5  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (condensation of, with aminothiophene derivative)
- IT 34570-16-6 102266-84-2  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (condensation of, with malononitrile)
- IT 107-95-9  
 RL: PROC (Process)  
 (knoevenagel condensation of aminodicyanobutenoate in presence of)
- IT 102266-58-0P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation and ether cleavage of)
- IT 86165-77-7P 102266-56-8P  
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
 (preparation and properties of)
- IT 921-76-6P 15828-10-1P 102266-57-9P 102266-59-1P 102266-60-4P  
 102266-61-5P 102266-62-6P 102266-63-7P 102266-64-8P 102266-65-9P  
 102266-66-0P 102266-67-1P 102266-68-2P 102266-69-3P 102266-70-6P  
 102266-71-7P 102266-72-8P 102266-73-9P 102266-74-0P 102266-75-1P  
 102266-76-2P 102266-77-3P 102266-78-4P 102266-79-5P 102266-80-8P  
 102266-81-9P 102266-82-0P 102266-83-1P 102282-91-7P 102291-59-8P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)



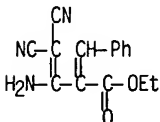
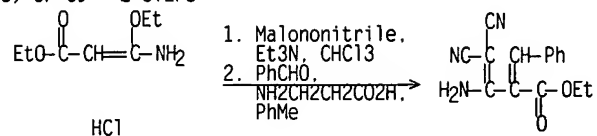
RX(35) OF 69 - 2 STEPS



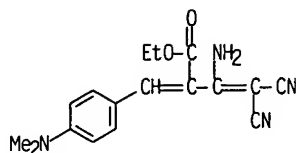
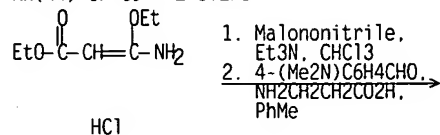
RX(36) OF 69 - 2 STEPS



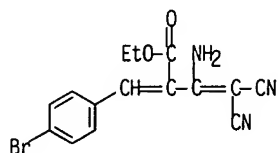
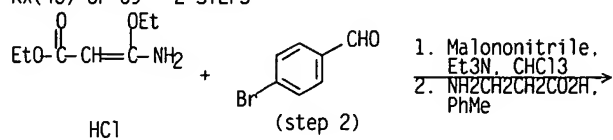
RX(43) OF 69 - 2 STEPS



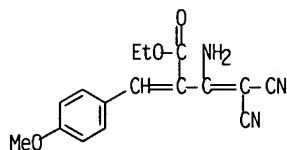
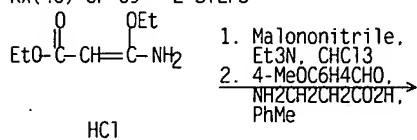
RX(44) OF 69 - 2 STEPS



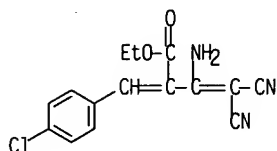
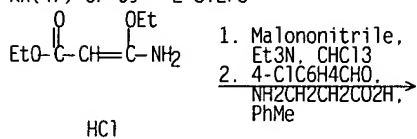
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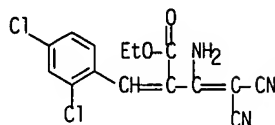
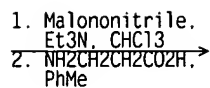
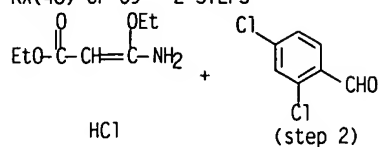
RX(46) OF 69 - 2 STEPS



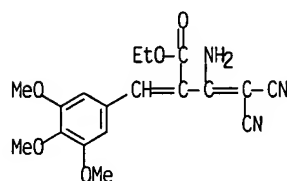
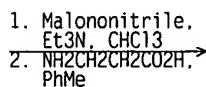
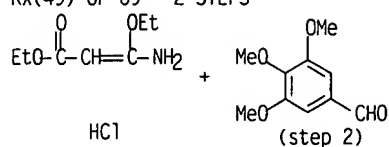
RX(47) OF 69 - 2 STEPS



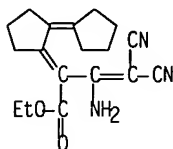
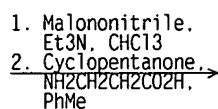
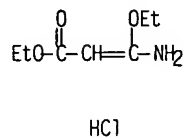
RX(48) OF 69 - 2 STEPS



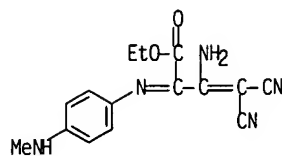
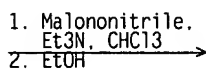
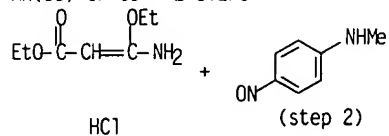
RX(49) OF 69 - 2 STEPS



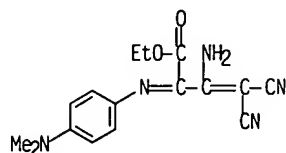
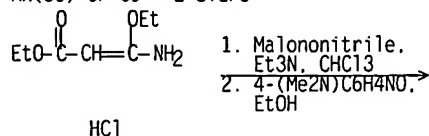
RX(54) OF 69 - 2 STEPS



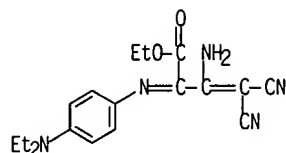
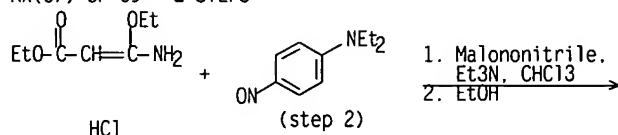
RX(55) OF 69 - 2 STEPS



RX(56) OF 69 - 2 STEPS



RX(57) OF 69 - 2 STEPS



L24 ANSWER 22 OF 28 CASREACT COPYRIGHT 2005 ACS on STN

AN 104:34047 CASREACT

TI Activated nitriles in heterocyclic synthesis: a novel synthesis of pyridazine, pyrimidine, pyridine and pyrano[4,3-b]pyridine derivatives

AU Mohareb, R. M.; Fahmy, S. M.

CS Fac. Sci., Cairo Univ., Giza, Egypt

SO Zeitschrift fuer Naturforschung, Teil B: Anorganische Chemie, Organische Chemie (1985), 40B(5), 664-8  
CODEN: ZNBAD2; ISSN: 0340-5087

DT Journal

LA English

AB RCOCH<sub>2</sub>C(NH<sub>2</sub>)=C(CN)CO<sub>2</sub>Et (I R = OEt) was treated with aromatic amines and aminoheterocyclic compds. to yield amide derivs. I (R = PhNH) was cyclized with aryldiazonium chloride, Cl<sub>3</sub>CCN, NaOMe, and cinnanonitriles and yielded resp. pyridazine, pyrimidine, pyridone, and pyrano[4,3-b]pyridine derivs.

CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))

ST amidation aminocyanopentenedioate arylamine; cyclocondensation aminocyanopentenedioate; pyridazinecarboxamide; pyrimidine cyanomethylene; pyridinone cyano; pyranopyridinecarbonitrile

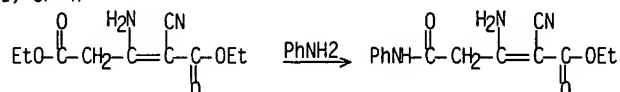
IT Cyclocondensation reaction  
(of aminocarbonylbutenoate with cinnamonitriles)IT Amidation  
(of aminocyanopentenedioate with aromatic or heterocyclic amines)IT Amides, preparation  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(heterocyclic, preparation of, from aminocyanopentenedioate)

IT 28447-79-2

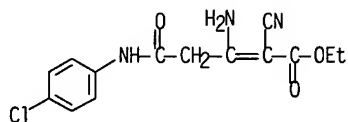
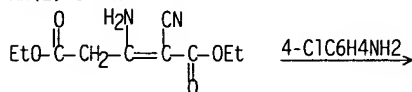
RL: RCT (Reactant); RACT (Reactant or reagent)

- (amidation of, with aromatic amines)
- IT 90-02-8, reactions  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(condensation of, with 4-(aminocarbonyl)-2-butenolate)
- IT 2025-40-3 2700-22-3  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(cyclization of, with 4-(aminocarbonyl)-2-butenolate)
- IT 545-06-2  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(cyclization of, with aminocyanopentenedioate)
- IT 99636-55-2P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and amidation of, with hydrazine)
- IT 99657-96-2P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and coupling of, with benzenediazonium chloride)
- IT 100-34-5P 2028-74-2P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and cyclization of, with aminocyanopentenedioate)
- IT 99636-48-3P 99636-60-9P 99636-61-0P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and cyclization of, with methoxide)
- IT 67231-68-9P 99636-49-4P 99636-50-7P 99636-51-8P 99636-52-9P  
99636-53-0P 99636-54-1P 99636-56-3P 99636-57-4P 99636-58-5P  
99636-59-6P 99636-62-1P 99659-02-6P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)
- IT 62-53-3, reactions 106-47-8, reactions 106-50-3, reactions 2010-06-2  
5049-61-6 28491-52-3  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with aminocyanopentenedioate)

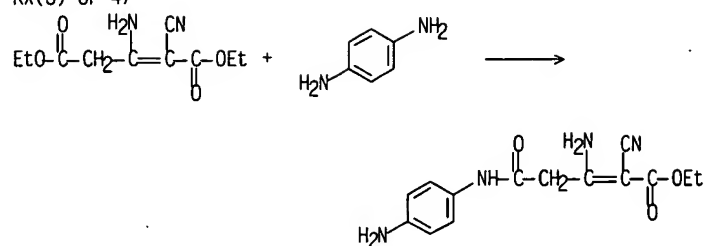
RX(1) OF 47



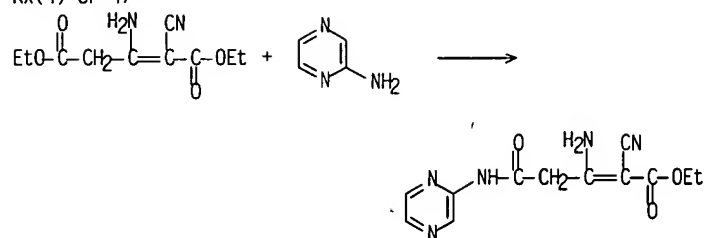
RX(2) OF 47



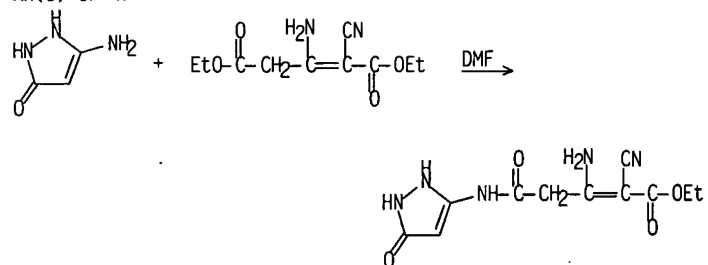
RX(3) OF 47



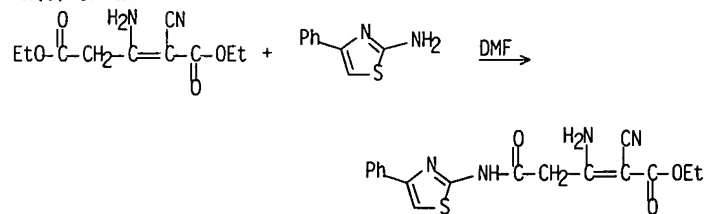
RX(4) OF 47



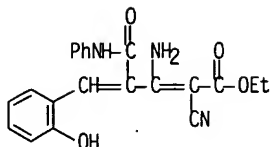
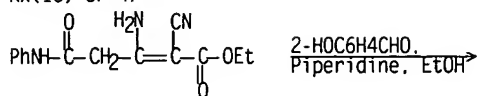
RX(5) OF 47



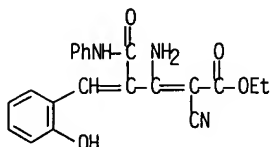
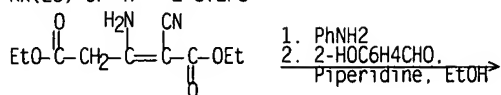
RX(6) OF 47



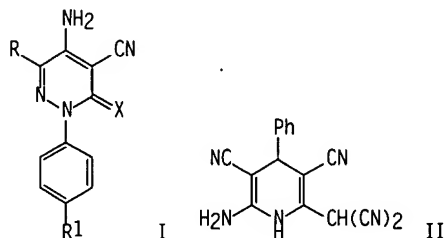
RX(16) OF 47



RX(25) OF 47 - 2 STEPS



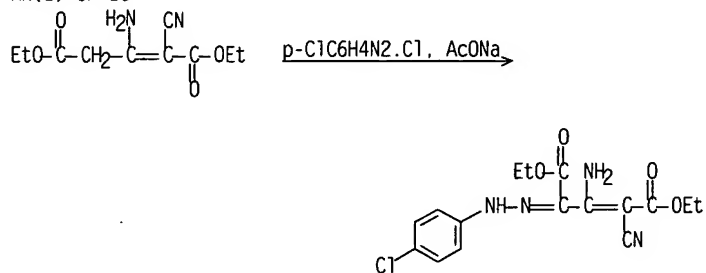
L24 ANSWER 23 OF 28 CASREACT COPYRIGHT 2005 ACS on STN  
 AN 102:185036 CASREACT  
 TI Activated nitriles in heterocyclic synthesis. Novel syntheses of pyrimidines and pyridines  
 AU Abed, N. M.; Ibrahim, N. S.; Fahmy, S. M.; Elnagdi, M. H.  
 CS Fac. Sci., Cairo Univ., Giza, Egypt  
 SO Organic Preparations and Procedures International (1985), 17(2), 107-14  
 CODEN: OPPIAK; ISSN: 0030-4948  
 DT Journal  
 LA English  
 GI



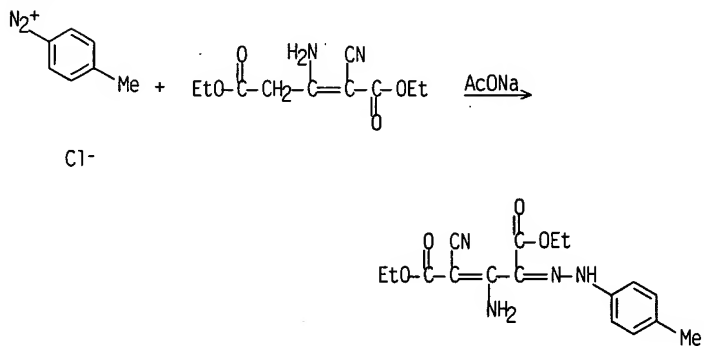
AB  $\text{RCH}_2\text{C}(\text{NH}_2):\text{CRCN}$  ( $\text{R} = \text{CO}_2\text{Et}$ , cyano) were treated with 4- $\text{R}_1\text{C}_6\text{H}_4\text{N}_2+\text{Cl}^-$  ( $\text{R}_1 = \text{Cl}$ , Me) to give the hydrazones 4- $\text{R}_1\text{C}_6\text{H}_4\text{NHN}:\text{CRC}(\text{NH}_2):\text{CRCN}$  which were cyclized on treatment with  $\text{NaOH-EtOH}$  to the pyridazines I ( $\text{X} = \text{O}$ , NH).  
 Reaction of  $\text{NCC}(\text{NH}_2):\text{C}(\text{CN})_2$  with  $\text{PhCH}:\text{C}(\text{CN})_2$  gave the pyridine II.  
 CC 28-15 (Heterocyclic Compounds (More Than One Hetero Atom))  
 Section cross-reference(s): 27  
 ST pyridazinone; pyridinedicarbonitrile; nitrile enamino arenediazonium

- IT 96122-10-0P 96122-11-1P 96122-12-2P 96122-13-3P 96122-17-7P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation and ring closure of)
- IT 74982-73-3P 74982-79-9P 82921-30-0P 96122-14-4P 96122-15-5P  
 96122-16-6P 96122-18-8P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)
- IT 868-54-2 28447-79-2  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, with arenediazonium chlorides)
- IT 60270-00-0  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, with cyanoacetate dimer)
- IT 2028-74-2 2028-84-4  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, with enamino nitriles)
- IT 2700-22-3  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, with malononitrile dimer)

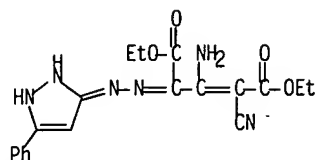
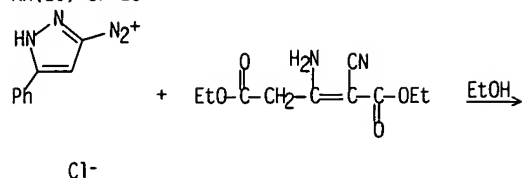
RX(1) OF 16



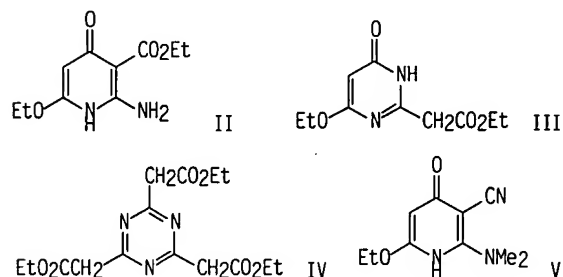
RX(2) OF 16



RX(10) OF 16



L24 ANSWER 24 OF 28 CASREACT COPYRIGHT 2005 ACS on STN  
 AN 99:21928 CASREACT  
 TI Self-condensation of ethyl 3-amino-3-ethoxypropenoate and related reactions  
 AU Ivanov, I.; Sulai, P.; Danchev, D.  
 CS Pharm. Fak., Med. Akad., Sofia, BG-1000, Bulg.  
 SO Liebigs Annalen der Chemie (1983), (5), 753-60  
 CODEN: LACHDL; ISSN: 0170-2041  
 DT Journal  
 LA German  
 GI



AB The cyclocondensation reaction of  $\text{EtOC}(\text{NH}_2):\text{CHCO}_2\text{Et}$  (I) (predominant tautomer shown) was catalyzed by acids ( $\text{F}_3\text{CCO}_2\text{H}$ ,  $\text{BF}_3$ ,  $\text{H}_2\text{SO}_4$ , 4-MeC<sub>6</sub>H<sub>4</sub>SO<sub>3</sub>H) and gave, via EtOH elimination, a mixture of pyridine, pyrimidine, and s-triazine derivs., e.g., II, III, and IV. To elucidate the course of the reaction, I was treated with  $\text{NCCH}_2\text{CO}_2\text{Et}$  and  $\text{CH}_2(\text{CN})_2$  to give  $\text{NCCR}:\text{C}(\text{NH}_2)\text{CH}_2\text{CO}_2\text{Et}$  ( $\text{R} = \text{CO}_2\text{Et}$ , cyano). Condensing I with  $\text{EtOC}(\text{NMe}_2):\text{CHCN}$  under self-condensation conditions gave chiefly pyridinone V.

CC 23-18 (Aliphatic Compounds)  
 Section cross-reference(s): 27, 28

ST aminoethoxypropenoate self condensation; cyclocondensation  
 aminoethoxypropenoate: propenoate aminoethoxy cyclocondensation; pyridine;  
 pyrimidinone; triazineacetate

IT Cyclocondensation reaction catalysts  
 (acids, for Et aminoethoxypropenoate)

IT Cyclocondensation reaction  
 (of Et aminoethoxypropenoate, pyridinone, pyrimidinone, and triazine  
 derivs. by)

IT 76-05-1, uses and miscellaneous 104-15-4, uses and miscellaneous

7637-07-2, uses and miscellaneous 7664-93-9, uses and miscellaneous

RL: CAT (Catalyst use); USES (Uses)

(catalysts, for cyclocondensation of Et aminoethoxypropenoate)

IT 39632-87-6

RL: RCT (Reactant); RACT (Reactant or reagent)

(cyclocondensation reactions of, catalysts for)

IT 86165-71-1P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation and ether cleavage of)

IT 28447-79-2P 86165-76-6P 86165-77-7P 86165-78-8P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)

IT 16654-91-4P 71470-18-3P 86165-70-0P 86165-72-2P 86165-73-3P

86165-74-4P 86165-75-5P

RL: SPN (Synthetic preparation); PREP (Preparation)

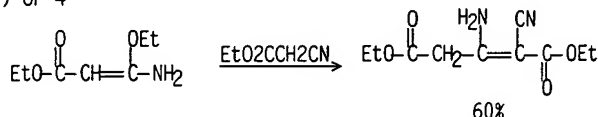
(preparation of, by acid-catalyzed cyclocondensation of Et aminoethoxypropenoate)

IT 105-56-6 109-77-3 34644-27-4

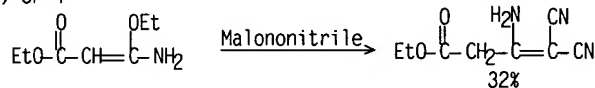
RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction of, with Et aminoethoxypropenoate)

RX(1) OF 4



RX(3) OF 4



L24 ANSWER 25 OF 28 CASREACT COPYRIGHT 2005 ACS on STN

AN 97:109951 CASREACT

TI Activated nitriles in heterocyclic synthesis: novel synthesis of pyridazines, pyridines, and isoxazoles

AU Fahmy, Sherif Mahmoud; Abed, Nosrat Mustafa; Mohareb, Rafat Milad; Elnagdi, Mohamed Hilmy

CS Fac. Sci., Cairo Univ., Giza, Egypt

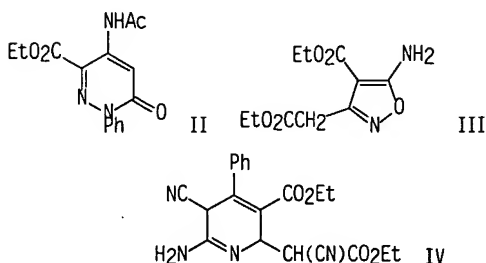
SO Synthesis (1982), (6), 490-3

CODEN: SYNTBF; ISSN: 0039-7881

DT Journal

LA English

GI

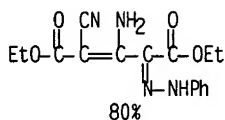
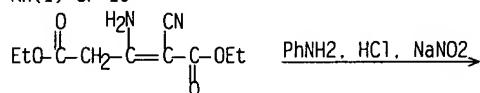


AB Pentenedioate ester EtO2CCH2C(NH2):C(CN)CO2Et (I) was converted to

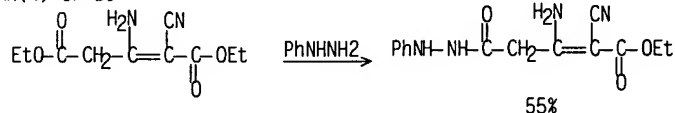
pyridazine derivative II, isoxazole derivative III, and pyridine derivative IV. Thus, PhNH<sub>2</sub> was diazotized, the product reacted with I to yield EtO<sub>2</sub>CC(:NNHPh)C(NH<sub>2</sub>):C(CN)CO<sub>2</sub>Et, and the latter was treated with Ac<sub>2</sub>O to give II. I, HONH<sub>2</sub>.HCl, and NaOAc in EtOH was refluxed to give III. IV was obtained from I and PhCH:C(CN)<sub>2</sub>.

- CC 28-15 (Heterocyclic Compounds (More Than One Hetero Atom))  
Section cross-reference(s): 27
- ST pyridazinecarboxylate amino; isoxazoleacetate amino; pyridineacetate cyano
- IT 100-63-0 302-01-2, reactions  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(condensation reaction of, with pyridazinecarboxylate ester derivative)
- IT 2700-22-3  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(cycloaddn. reaction of, with aminopentenedioate ester derivative)
- IT 5470-11-1  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(cyclocondensation-cycloaddn. reaction of, with aminocyanopentenedioate ester)
- IT 62-53-3, reactions  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(diazotization of, and reaction of product with pentenedioate ester derivative)
- IT 82754-63-0P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and cyclocondensation reaction of)
- IT 82754-64-1P 82754-65-2P 82754-66-3P 82754-67-4P 82754-68-5P  
82754-69-6P 82754-70-9P 82754-71-0P 82754-72-1P 82754-73-2P  
82867-18-3P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)
- IT 79407-65-1  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reactions of, with benzenediazonium salt, benzyldenemalononitrile and hydroxylamine, heterocycles from)

RX(1) OF 10



RX(4) OF 10



L24 ANSWER 26 OF 28 CASREACT COPYRIGHT 2005 ACS on STN

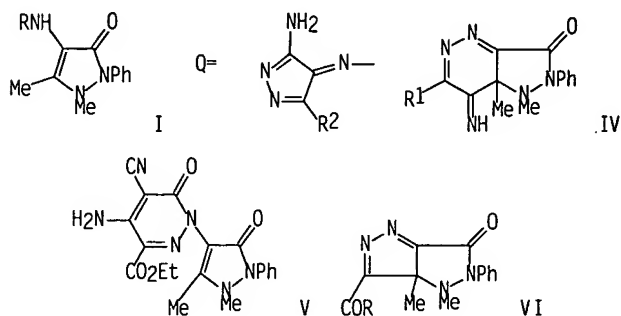
AN 97:92189 CASREACT

TI Reactions with heterocyclic diazonium salts: novel synthesis of pyrazolo[4,3-c]pyridazines and of pyrazolo[4,3-c]pyrazoles

AU Elmagdi, Mohamed Hilmy; Elfahham, Hassan Attia; Elmoghayar, Mohamed Rifaat Hamza; Sadek, Kamal Usef; Elgemeie, Galal Eldin Hamza

CS Dep. Chem., Minia Univ., Minia, Egypt

SO Journal of the Chemical Society, Perkin Transactions 1: Organic and  
Bio-Organic Chemistry (1972-1999) (1982), (4), 989-91  
CODEN: JCPRB4; ISSN: 0300-922X  
DT Journal  
LA English  
GI



AB Diazotized pyrazolone I (R = H) coupled with  $R_1CH_2CN$  ( $R_1$  = cyano,  $CO_2Et$ ,  $Me:NH$ ) and  $Z-EtO_2CCH_2C(NH_2):C(CN)CO_2Et$  in  $EtOH-NaOAc$  at room temperature for 2 h to give the corresponding cyanohydrazone I [R =  $N:C(CN)R_1$  (II),  $N:C(CO_2Et)C(NH_2):C(CN)CO_2Et$  (III)] in 66-91% yield. Cyclocondensation reactions of II with  $N_2H_4$  in refluxing  $EtOH$  for 3 h gave pyrazolylidenehydrazinopyrazoles I (R = Q;  $R_2$  =  $NH_2$ , OH, Me) in 81, 85, and 88% yield, resp. On refluxing in acidic  $EtOH$  for 2 h II ( $R_1$  = cyano,  $CO_2Et$ ,  $Me:NH$ ) cyclized to give 45-78% pyrazolopyridazines IV ( $R_1$  = cyano,  $CO_2Et$ ,  $Me:NH$ ), resp. III cyclized to give 84% pyridazine V on refluxing in  $EtOH$ . Reaction of diazotized I (R = H) with  $RCOCHClCOMe$  (R = Me,  $OEt$ ) in  $EtOH$  at room temperature for 2 h gave the corresponding pyrazolopyrazolones VI in 74 and 53% yield, resp.

CC 28-8 (Heterocyclic Compounds (More Than One Hetero Atom))

Section cross-reference(s): 23

ST diazotization coupling aminodimethylphenylpyrazolone nitrile;  
oxypyrazolylhydrazone cyanoalkanal prepn cyclization; hydrazine  
cyclocondensation cyanoalkanal oxypyrazolylhydrazone;  
pyrazolylidenehydrazinopyrazolone; pyrazolopyridazine;  
pyrazolylpyridazine; chloroalkanedione coupling cyclization  
aminodimethylphenylpyrazolone; pyrazolopyrazole; pyrazolone amino  
diazotization coupling nitrile

IT Nitriles, reactions

RL: RCT (Reactant); RACT (Reactant or reagent)

(coupling reactions of, with diazotized aminodimethylphenylpyrazolone)

IT Cyclocondensation reaction

(of cyanoalkanal oxypyrazolylhydrazones with hydrazines,  
pyrazolylidenehydrazinopyrazoles by)

IT Ring closure and formation

(of cyanoalkanal oxypyrazolylhydrazones, pyrazolopyridazines by)

IT Coupling reaction

(of diazotized aminodimethylphenylpyrazolone with nitriles and  
chloroalkanones)

IT Cyclocondensation reaction

(intramol., of di-Et (oxypyrazolylhydrazino)cyanoaminopentadienoate,  
pyrazolylpyridazine by)

IT 105-56-6 1118-61-2 4341-85-9 28447-79-2

RL: RCT (Reactant); RACT (Reactant or reagent)

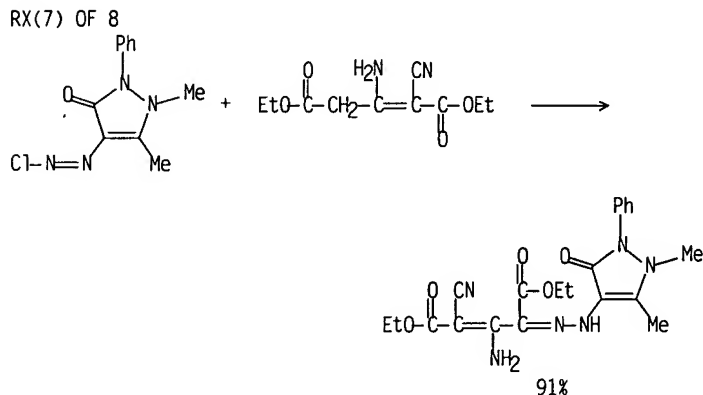
(coupling reaction of, with diazotized aminodimethylphenylpyrazolone)

IT 609-15-4 1694-29-7

RL: RCT (Reactant); RACT (Reactant or reagent)

(coupling-cyclization reaction of, with diazotized

- aminodimethylphenylpyrazolone)
- IT 302-01-2, reactions  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(cyclocondensation reaction of, with cyanoalkana  
oxopyrazolylhydrazones)
- IT 83-07-8  
RL: PRP (Properties)  
(diazotization and coupling of, with methylenenitriles and  
chloroalkanones)
- IT 82315-81-9P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)  
(preparation and intramol. cyclocondensation reaction of,  
pyrazolylpyridazine by)
- IT 82315-72-8P 82315-73-9P 82315-74-0P 82315-75-1P 82315-76-2P  
82315-77-3P 82315-78-4P 82315-79-5P 82315-80-8P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)
- IT 81437-82-3P 81437-83-4P 82315-71-7P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)  
(preparation, cyclization, and cyclocondensation reaction of, with  
hydrazine)



- L24 ANSWER 27 OF 28 CASREACT COPYRIGHT 2005 ACS on STN
- AN 96:34716 CASREACT
- TI .beta...beta.-Diaclylenamines and -enols. 9. Synthesis of aminomethylene  
derivatives of open-chain methylene acidic compounds
- AU Wolfbeis, Otto S.
- CS Inst. Org. Chem., Univ. Graz, Graz, A-8010, Austria
- SO Chemische Berichte (1981), 114(11), 3471-84  
CODEN: CHBEAM; ISSN: 0009-2940
- DT Journal
- LA German
- AB RR1C:CR2NR3R4 (R = cyano, CO2Me, CO2Et, Ph, Bz, COCH2C1, CONHPh, Ac; R1 =  
NO2, C6H4NO2-4, SO2Ph, Bz, CONH2, CONHPh, CO2Me, CO2Et, cyano, Ph,  
CONHCONH2; R2, R3 = H, Me; R4 = Ph, CH2Ph, 1-adamanty1, CONHMe,  
2-benzothiazoly1, 2-pyridyl) were prepared by treating RR1CH2 with R2C(OMe)3  
or R2C(OEt)3 and R3R4NH. Similar reaction of HO2CCH2R5 (R5 = CO2H, cyano,  
SO2Ph) with R2C(OMe)3 and R4NH2 gave (R4NH)2C+R2 -O2CCH2R5.
- CC 25-4 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
- ST enamine diacyl; methylene active amine orthoalkanoate
- IT Enamines

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of, from amines, orthoalkanoates, and methylene-active compds.)

IT 15568-92-0

RL: RCT (Reactant); RACT (Reactant or reagent)  
(hydrolysis of)

IT 80421-14-3P 80421-16-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)  
(preparation and cyclization of)

IT 1202-48-8P 1209-08-1P 2305-54-6P 6123-64-4P 6123-68-8P  
6123-71-3P 7144-24-3P 13820-19-4P 24115-28-4P 26533-49-3P  
26978-72-3P 51991-92-5P 54925-91-6P 75544-71-7P 80420-91-3P  
80420-92-4P 80420-93-5P 80420-94-6P 80420-95-7P 80420-96-8P  
80420-97-9P 80420-98-0P 80420-99-1P 80421-00-7P 80421-01-8P  
80421-02-9P 80421-03-0P 80421-04-1P 80421-05-2P 80421-06-3P  
80421-07-4P 80421-08-5P 80421-09-6P 80421-10-9P 80421-11-0P  
80421-12-1P 80421-13-2P 80421-15-4P 80421-17-6P 80422-10-2P  
80430-68-8P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

IT 1830-54-2 2651-09-4

RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with aniline and trimethoxymethane)

IT 122-51-0 149-73-5 1445-45-0

RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with methylene-active compds. and amines)

IT 62-53-3, reactions 100-46-9, reactions

RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with methylene-active compds. and orthoalkanoates)

IT 100-61-8, reactions 136-95-8 504-29-0 598-50-5 768-94-5

RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with methylene-active compds. and trimethoxymethane)

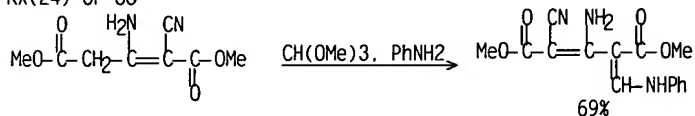
IT 102-01-2 105-34-0 105-56-6 107-91-5 109-77-3 451-40-1 555-21-5  
614-16-4 614-21-1 621-03-4 622-42-4 2483-57-0 5445-26-1  
7605-28-9 13218-13-8 32807-28-6 53341-66-5 76311-94-9

RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with orthoalkanoate and amines)

IT 141-82-2, reactions 372-09-8 3959-23-7

RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with orthoalkanoates and amines)

RX(24) OF 38



L24 ANSWER 28 OF 28 CASREACT COPYRIGHT 2005 ACS on STN

AN 94:30680 CASREACT

TI Reaction of 3-amino-2-benzoylcrotonate esters with phosgene

AU Ward, Frederick E.; Buckler, Robert T.

CS Chem. Dep., Miles Lab., Inc., Elkhart, IN, 46515, USA

SO Journal of Organic Chemistry (1980), 45(23), 4608-11

CODEN: JOCEAH; ISSN: 0022-3263

DT Journal

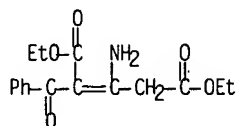
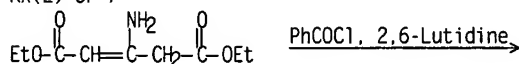
LA English

AB COC12 (I) in the presence of 2,6-lutidine, reacts with alkyl esters of 3-amino-2-benzoylcrotonic acid to give as major products 1,3-oxazin-2-ones, formally derived from the reaction of 2 equivalent of amino ester with 2 and 3 equivalent of I. Et 3-amino-2-benzoyl-2-pentenoate reacts with I-2,6-lutidine to give a 1,3-oxazin-2-one derived from the reaction

of 1 equivalent of I and 1 equivalent of amino ester. Di-Et 3-amino-2-benzoylglutaconate reacts with COCl<sub>2</sub>-2,6-lutidine to give both a "1:1" 1,3-oxazin-2-one and a 4-aminopyrone.

- CC 28-14 (Heterocyclic Compounds (More Than One Hetero Atom))  
Section cross-reference(s): 25, 27
- ST phosgene cyclocondensation aminobenzoylcrotonate; benzoylcrotonate amino phosgene cyclocondensation; crotonate aminobenzoyl phosgene cyclocondensation; oxazinone; pyrone amino; lutidine cyclocondensation catalyst
- IT 98-88-4  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(benzoylation by, of di-Et aminoglutaconate)
- IT 54889-50-8  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(benzoylation of, with benzoyl chloride)
- IT 75-44-5  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(cyclocondensation of, with aminobenzoylcrotonate esters)
- IT 21486-64-6 74947-57-2  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(cyclocondensation of, with phosgene, in presence of lutidine)
- IT 74947-62-9P 74947-65-2P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and cyclocondensation of, with phosgene, in presence of lutidine)
- IT 74947-67-4P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and hydrogenation of, ring cleavage in)
- IT 74947-55-0P 74947-56-1P 74947-58-3P 74947-59-4P 74947-60-7P  
74947-61-8P 74947-63-0P 74947-64-1P 74947-66-3P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)
- IT 108-03-2  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with Et pyrrolidinylcinnamate and Ph isocyanate)
- IT 103-71-9, reactions  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with Et pyrrolidinylcinnamate and nitropropane)
- IT 53256-23-8  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with propane and Ph isocyanate)

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